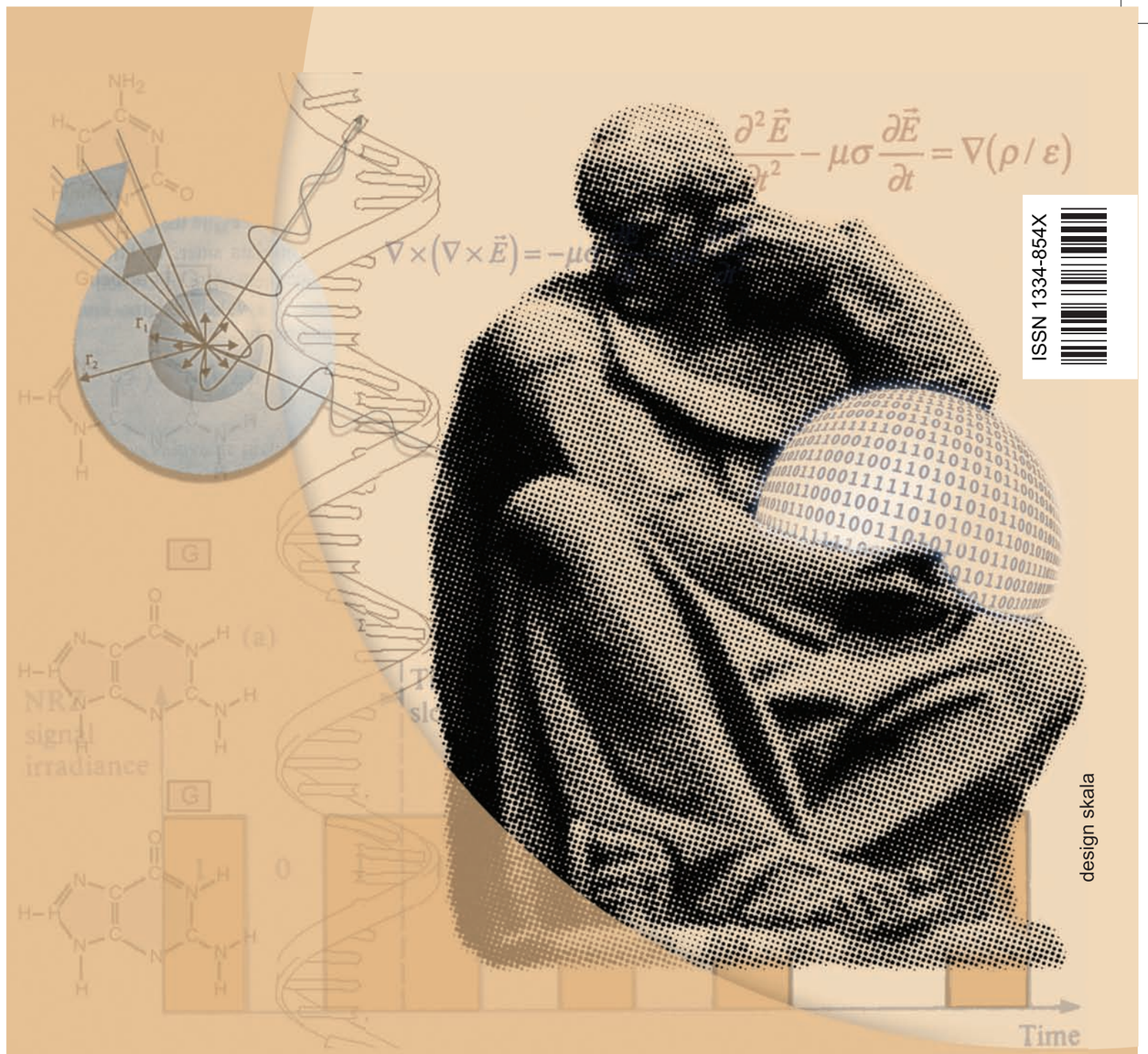
Ruđer Bošković Institute

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

RBI Annual Report 2009



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Ruđer Bošković Institute

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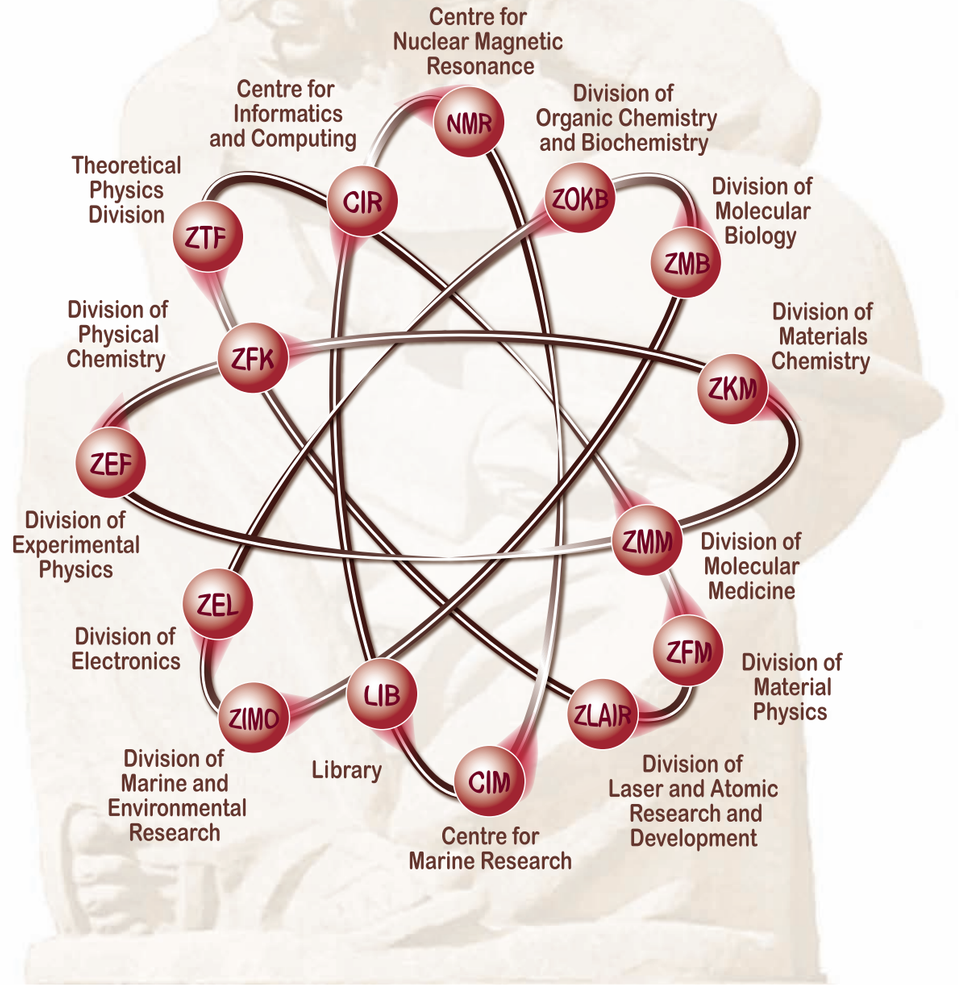
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Contents

Dear reader,

Welcome to the 2009 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 2009. 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 RBI is the largest Croatian research centre for basic sciences, participating also in science applications and higher education. The multidisciplinary character of the Institute is reflected through the different research fields in physics, chemistry, oceanography (including marine and environmental research and geosciences), biology, biomedicine, computer science and electronics/engineering. At the end of 2009, the Institute had a total of 887 employees. This included 308 scientists, 68 postdoctoral researchers, 172 Ph.D. students, 112 support scientists and technicians, 65 administrative staff, 141 maintenance and security staff, and 21 library and IT staff.

ORGANIZATION OF THE INSTITUTE

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

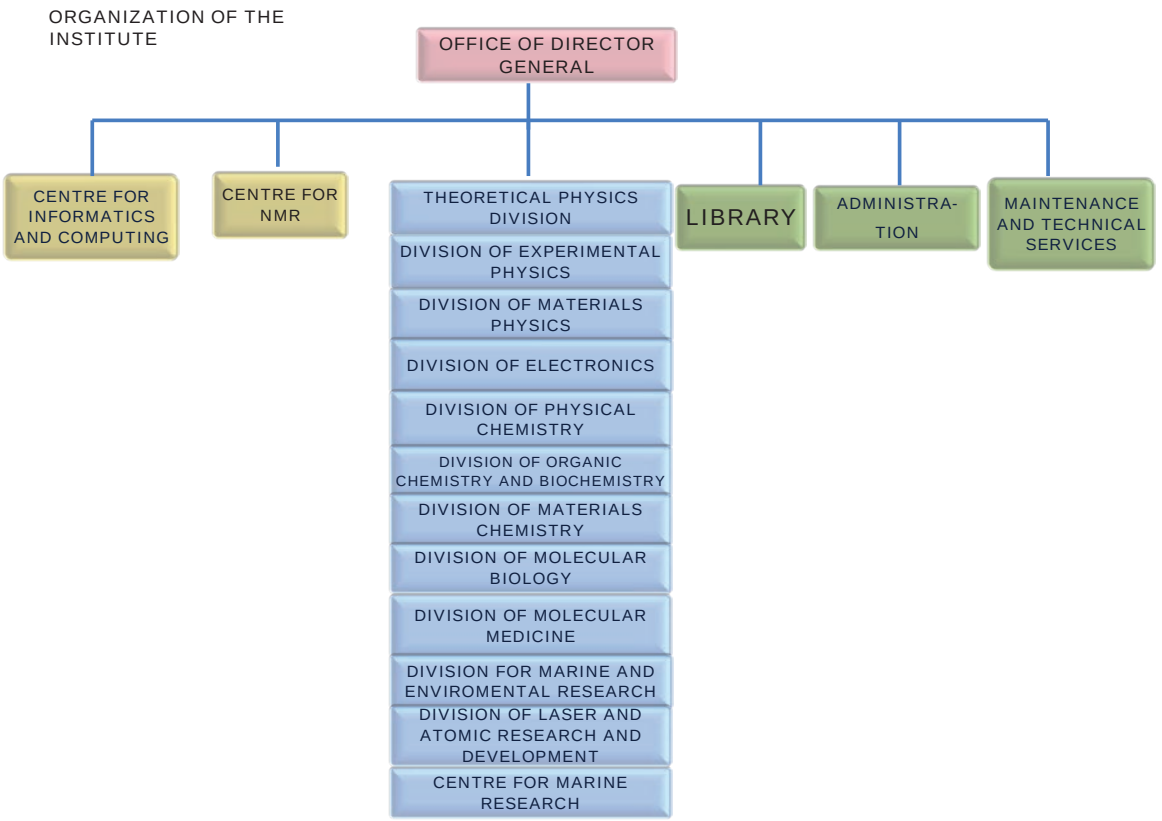


Figure 1. The organizational structure of the RBI

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.

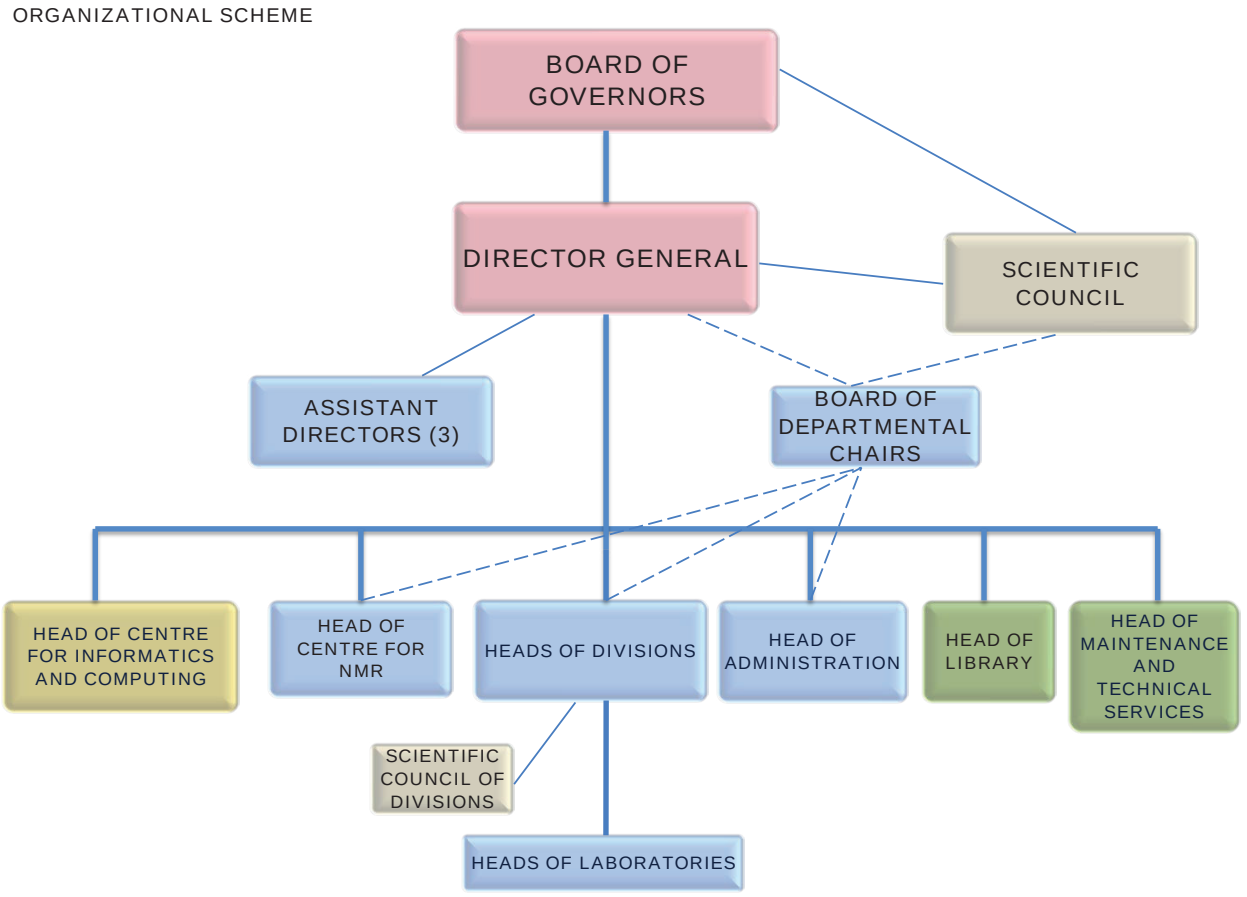


Figure 2. The administrative structure of the RBI

Director General: Mladen Žinić
(until March 3rd, 2009)
Acting Director: Jaroslav Horvat
(from March 4th to May 14th, 2009)
Director General: Danica Ramljak
(from May 15th, 2009)
Head of the Scientific Council: Neven Bilić
Chairman of the Board of Governors:
Slavko Krajcar

International Scientific Board:

Jean-Marie Lehn, Laboratoire de Chimie Supramoléculaire, ISIS/ULP, France
Harold Kroto, University of Sussex, UK
Egon Matijević, Clarkson University, NY, USA
Helmut Schwarz, Technische Universität Berlin, Germany
Fritz Vögtle, Universität Bonn, Germany
Robert Blinc, Jozef Stefan Institute, Ljubljana, Slovenia
Jonathan R. Ellis, CERN, Switzerland
Anthony R. Peaker, University of Manchester, UK
Bogdan Povh, MPI für Kernphysik, Heidelberg, Germany
Roberto D. Peccei, UCLA, Los Angeles, CA, USA
Fernando Azorin, Institute of Molecular Biology of Barcelona, Spain
Bernd Kaina, Institut für Toxikologie, Mainz, Germany
Werner E. G. Müller, Johannes Gutenberg Universität, Mainz, Germany
Miroslav Radman, Université René Descartes-Paris V, France
Jürgen Soll, Ludwig-Maximilians-Universität München, Germany
Vito Turk, Jozef Stefan Institute, Ljubljana, Slovenia
Joseph Schlessinger, Yale University School of Medicine, CT, USA
Hans Joachim Seitz, Universität Hamburg, Germany
Davor Solter, MPI für Immunbiologie, Freiburg, Germany
Peter J. Stambrook, University of Cincinnati Medical Center, OH, USA
Rudolf Zechner, Institute for Molecular Biosciences, Graz, Austria
Farooq Azam, University of California, San Diego CA, USA
Walter Giger, Swiss Federal Institute for Aquatic Sciences and Technology, Dübendorf/Zürich, Switzerland
Thomas C. Malone, OceanUS Office for Integrated and Sustained Ocean Observations, Arlington, VA, USA
Nadia Pinardi, University of Bologna, Ravenna, Italy

ACTIVITIES

Fundamental research

The total number of research articles published by RBI scientists in 2009 was 559. Amongst these, 434 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 2009 are to be found in the subsequent sections of this report. Nevertheless, we present here a small selection of highlights in order to convey a general impression of the kind of research carried out at the Institute.

Scientists from the Division of Molecular Biology made advances in understanding the efficiency of photosynthetic energy conversion. Their study was focused on the TROL protein of plant photosynthetic membranes that interacts with a flavoenzyme (FNR) involved in the final step of the photosynthetic electron flow. Plants devoid of the TROL protein exhibited decreased electron flow, proving the importance of the target protein for efficient photosynthesis.

Studies of biomineral encrustation on a 2,000-year-old bronze sculpture of the famed

ancient Greek athlete Apoxyomenos, carried out by scientists at the Centre for Marine Research in Rovinj, have shown how marine organisms may provide passivating layers for the protection of metal objects and may provide new understanding of how to prevent metal corrosion or develop safer ways to permanently store nuclear waste.

Quantum dots ordered in regular lattices, called quantum dot superlattices, have been under investigation in the Division of Materials Physics because they offer numerous possibilities for the creation of novel materials. While this phenomenon has been satisfactorily explained in crystalline materials, RBI scientists have now observed the spontaneous formation of quantum dot superlattices in amorphous systems. These superlattices exhibit interesting collective behavior due to self-organized regular growth, which was also simulated by a theoretical model. The discovery paves the way for further development of quantum-dot arrays in amorphous matrices.

On the other end of the spectrum, scientists from the Division of Experimental Physics studied hadronic axions, which may be produced in the Sun. Using a HPGe detector, the team searched for the axions by an axioelectric effect and, though their efforts, were able to place a conservative upper limit on the hadronic axion mass.

Projects and other revenue

The RBI has 138 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 the RBI has 5 and 10 active projects, respectively. The Institute is involved with more than 100 international projects (including: 8 FP7, 5 FP6, 5 IAEA, 3 NATO, 1 INTERREG, 1 ERITRACK, and 77 bilateral projects), as well as 72 applied and technological contracts (including 2 funded by HIT, 2 by HITRA, 1 by VIP, and 1 by BICRO). The total financial value of these projects can be seen in Table 1, as well as the funding trends since 2005.

REVENUE	2005	2006	2007	2008	2009
Domestic projects funding (basic projects, equipment, JADRAN, UKF, Croatian Science Foundation, HITRA...)	4.720.646	4.217.961	6.185.637	5.553.639	3.975.440
International projects funding (FP, NATO, IAEA...)	92.576	518.819	623.877	834.643	1.517.186
External contracts (comercial contracts)	1.885.167	1.747.505	1.969.845	2.315.107	2.222.115
Donations and other funding	221.607	380.193	976.465	396.681	522.100
Funding from Ministry of Sciences, Education and Sports (MSES)	15.816.658	17.117.556	18.968.319	21.852.542	20.808.470
Total	**22.736.654**	**23.982.034**	**28.724.143**	**30.952.612**	**29.045.311**

Table 1. The RBI budget (2005-2009)

Table 1 also shows that largest non-competitive source of revenue continues to be derived from the Ministry of Science, Education and Sports, which directly contributed some € 20,8 M in 2009. 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 was reduced in 2009. Thus despite the increase in international project funding observed during 2009, the total RBI revenue was reduced by almost € 2 M, in comparison to 2008.

Organization of international **conferences**

As in previous years, the RBI continued to support the organization of numerous international and domestic conferences. For example, The Exploratory Workshop on ‘’How to Constrain the High Density Symmetry Energy’’ sponsored by European Science Foundation (ESF) and organized for the RBI Laboratory for Nuclear Physics by Zoran Basrak was held from 16th to 18th October 2009 in Zagreb. The international nuclear physics conference "Nuclear Structure and Dynamics" organized by the RBI Laboratory for Nuclear Physics and the University of Zagreb and co-chaired by S. Szilner was held from 4th to 8th May 2009 in Dubrovnik. In the context of an FP6 project and also with support from the ESF, The 3rd Adriatic Meeting on Computational Solutions in the Life Sciences, in, Croatia, was organized jointly by Sanja Tomić, Darko Babić, and Nađa Došlić (Division of Physical Chemistry) and David Smith (Division of Organic Chemistry and Biochemistry) from the 1st to the 5th of September 2009 in Primošten. The 10th International School on Biophysics was organized by Igor Weber and Ksenija Zahadraka from the 15th to the 30th of September 2009 in Rovinj.

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

Awards and Recognition

As in previous years, RBI the achievements of RBI scientists were also recognized through numerous awards. For example, Zvonimir Maksić, from the Division of Organic Chemistry and Biochemistry, received the National Science Award of the Republic of Croatia for the Lifetime Achievements in the field of Natural Sciences. The Annual Croatian State Award for Biomedicine was presented to Nela Pivac, from the Division of Molecular Medicine, for her research in the field of biomedicine and especially her significant achievements in research studying the molecular basis and treatment of psychiatric disorders. The Annual Croatian State Award for Science was given to Ante Graovac, from the Centre for NMR, for discovery and development of novel methods of mathematical chemistry and their applications to various fields of chemistry and material sciences. Branka Medved Rogina, from the Division of Electronics, was awarded the Croatian Academy of Engineering Annual Award 'Richard Podhorsky' for 2008, for distinguished scientific contribution in the development and application of high resolution timing measurement methods and testing of microelectronics and optoelectronics devices, with an emphasis on using new electronic technologies in the Republic of Croatia and beyond. Nikola Basarić, from the Division of Organic Chemistry and Biochemistry, received the Leopold Ružička award for young scientists of the Croatian Chemical Society.

Education

Table 2 shows the significant participation of scientists from the Institute in programs of higher education in Croatia. Undergraduate and graduate courses were provided at

Number of undergraduate courses	75
Number of graduate courses	81
Number of Ph.D. courses	211
Mentoring of B.Sc. theses	47
Mentoring of specialist postgraduate studies	6
Mentoring of specialist Ph.D. studies	40
Organisation and leading of courses in specialist studies	2

Table 2. Number of the RBI held courses and theses

universities in Zagreb, Split, Rijeka, Zadar, Osijek, Pula, and Dubrovnik. An active role in mentoring is also visible in Table 2, with the number of B.Sc. theses supervised at the RBI almost double the level achieved in 2008.

Table 3 shows the distribution of the courses provided across the different RBI Divisions and Centres. While the Division of Molecular Medicine was the most active in this respect, almost all Divisions actively participated in the provision of courses to Croatian students.

Intellectual Property

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

Department	Undergraduate study	Specialist postgraduate study + MSc study	PhD study	Organization of specific studies
OKB	6	-	**3**	-
ZKM	1	1MSc	**-**	-
ZFK	1	-	**1**	-
ZIMO	4	2MSc	**9**	-
NMR	-	-	**-**	-
CIR	3	-	**-**	study
LAIR	-	-	**-**	-
ZMM	14	3MSc	**6**	-
ZMB	9	-	**3**	-
ZTF	-	-	**3**	-
ZEF	8	-	**4**	-
ZFM	4	-	**1**	study
CIM	1	1MSc	**1**	-

Table 3. Number of the RBI held undergraduate, specialist postgraduate (M.Sc.) courses and Ph.D. courses and specific courses

the protection of intellectual property and its commercialization. In this context, various specific activities have been initiated and realized over the last few years. For example, we have established a company under the name Rudjer Innovations Ltd. This company, which is wholly owned by the RBI, engages in activities related to protection and commercialization of knowledge arising from the RBI, other academic organizations, companies, and private persons.

Two patents arising from work at Ruđer Bošković Institute were granted in 2009; one European patent (EP 1786763 from Mirjana Maksić and Zoran Glasovac) and one United States patent (No. 7,658,850 from Dubravka Hršak and Maja Havriluk). Rudjer Innovations also filed 6 new patent applications on behalf of the Institute in 2009 - 5 Croatian national applications and 1 international patent application. Furthermore, 3 existing Croatian national patent applications entered the international (PCT) phase in 2009 and 6 patent applications were filed in the national phase of patent protection in 2009 (two in the EU, three in the USA and one in Canada).

Table 4. Publication results of fundamental research projects at RBI

Field of Science	Project Title	Principal Investigator	Number of CC Articles Published in 2009 (Journa articles and review articles published in CC journals in 2009)
Biology - 75	Regulatory mechanisms of photosynthesis and plastid differentiation	Hrvoje Fulgosi	5
	Molecular regulation of plant development	Branka Salopek-Sondi	8
Physics - 87	Physic and application of nanostructures and bulk matter	Krešimir Furić	14
	Nuclear structure and reactions: experimental approach	Suzana Szilner	11
	Fundamental interactions in elementary particle physics and cosmology	Branko Guberina	9
	Basic properties of nanostructures and defects in semiconductors and dielectrics	Branko Pivac	10
	Massive neutrinos and astroparticles: from particle physics to cosmology	Ante Ljubičić	11
	Ion beam interactions and nanostructures	Milko Jakšić	13
	Heavy-ion physics	Zoran Basrak	10
	Thin films of novel amorphous or nanostructured materials	Nikola Radić	8

	Tanki filmovi legura silicija na prijelazu iz amorfne u uređenu strukturu	Davor Gracin	11
Earth science - 64	Nature of organic matter, interaction with traces and surfaces in environment	Zlatica Kozarac	10
	Interactions of trace metal species in an aquatic environment	Ivanka Pižeta	9
	Stanične promjene u vodnih organizama pobuđene metalima	Biserka Raspor	6
	Radionuclides and trace elements in environmental systems	Delko Barišić	5
Chemistry - 74	Synthesis and microstructure of metal oxides and oxide glasses	Svetozar Musić	11
	NMR Spectroscopy and Modelling of Bioactive Molecules	Dejan Plavšić	15
	Molecular structure and dynamics in systems containing paramagnetic particles	Boris Rakvin	6
	Electroanalytical research on microcrystals and traces of dissolved substances	Milivoj Lovrić	7
	Protein-ligand međudjelovanja na atomnoj razini	Marija Luić	11
	Self-Assembly in gels and synthesis of functional hybrid materials	Mladen Žinić	8
	Dizajn, sinteza i ispitivanje interakcija malih molekula s DNA, RNA i proteinima	Ivo Piantanida	9
Computer science - 27	Multispectral data analysis	Ivica Kopriva	9
Fundamental medical sciences - 167	The role of different cell death responses to DNA-damage treatment	Marijeta Kralj	9
	Molecular characteristic of myofibroblasts derived from Dupuytren's contracture	Krešimir Pavelić	7
	Pharmacogenomics and proteomics of serotonergic and catecholaminergic system	Dorotea Muck-Šeler	8
	Molecular basis and treatment of psychiatric and stress related disorders	Nela Pivac	8
	Lipids, free radicals and their messengers in integrative oncology	Neven Žarković	7
	Gene therapy of tumors by modulating the molecules of immune system	Jasminka Pavelić	7

	Aberrant DNA methylation in HPV associated lesions	Magdalena Grce	4
	Molecular genetics and pharmacogenetics of gastrointestinal tumors	Sanja Kapitanović	4
Agriculture - 156	Substanična biokemijska i filogenetska raznolikost tkiva riba, rakova i školjaka	Rozelinda Čož-Rakovac	3

Table 4. shows the projects led by RBI scientists which are ranked among the top 15% in the country, according to the Croatian Scientific Bibliography (CROSBI). The number of projects in a particular field of science is taken from the official list of the projects provided by the Ministry of Sciences, Education and Sport. The ranking is performed by the total number of articles associated with a particular project among the projects that begun in 2007 – only research articles published in journals cited in Current Contents were counted (web address: http://bib.irb.hr/statistika?sto=p&period=2009&chset=ASCII&lang=EN). The number of articles is the total number of scientific papers published in this particular project in 2009, up until February 9th, 2010. The limitation of the table is that it does not include an average journal impact factor, the number of researchers/students working on the project, and the financial support of the projects.

Theoretical Physics Division

http//thphys.irb.hr

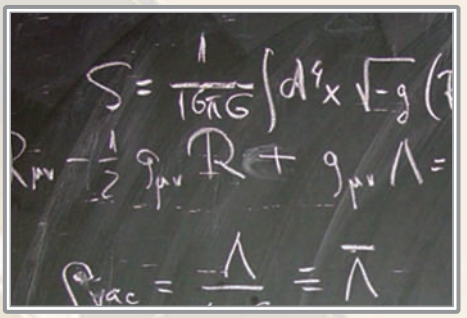
ZTF

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



OVERVIEW OF THE DIVISION

The research performed in the Division is mainly concerned with the theoretical investigation of high-energy physics, such as particle physics, general and mathematical physics, astroparticle physics and cosmology. In addition, there is substantial research activity in condensed matter physics. In 2009, the members of the Division continued to be involved in lecturing at the University of Zagreb and a number of students completed their Ph. D. theses.

TOP ACHIEVEMENTS

The solution of the cosmological constant problem?

A cosmological model containing a cosmological constant of arbitrary size and sign and a component with an inhomogeneous equation of state is introduced. It is shown that the asymptotic expansion of the universe in the model corresponds to the universe with a small effective cosmological constant comparable to the observed value. The effect of a large cosmological constant in the model is dynamically relaxed in a robust way without fine-tuning of model parameters. Thus the proposed model represents the solution of the notorious “old” cosmological constant problem. It is shown that introduction of a relaxation mechanism could be realized in modified gravity theories (Štefančić, 2009).

Unification of dark energy and dark matter

A k-essence type of theory similar to tachyon condensate models has been examined as a potential model for dark energy/matter unification. The general relativistic spherical model has been extended to incorporate the effects of both pressure and the acoustic horizon. It has been demonstrated that an initially perturbative k-essence fluid evolves into a mixed system containing a cold dark matter-like gravitational condensate in significant quantities (Bilić et al., 2009).

CP violation and the 4th generation

Within the Standard model with the 4th generation quarks b' and t' CP-violating flavor changing neutral current processes (t -> cX; b'-> sX, b'-> bX, t'-> cX, and t'-> tX, with X = Z, H, gamma, g) have been analyzed by constructing and employing global, unique fit for the 4th generation mass mixing matrix CKM4 at 300 < m_t' < 700 GeV. It has been found that our fit produces the CP partial rate asymmetry dominance for b'-> s(Z,H,gamma,g) decays, up to 90%, depending on the mode and m_t'. Also, a relatively large a_CP(t -> c g) ~ 15 (10)% for t' running in the loops with the mass m_t'= 650(500) GeV has been obtained. There are fair chances that the 4th generation quarks will be discovered at Tevatron or LHC and that some of the calculated decay rates and CP asymmetries will be measured (Eilam et al., 2009).

Renormalization of Hamiltonian QCD

Renormalization of QCD in the Coulomb gauge using the Hamiltonian formalism has been studied to one-loop order. Divergences occur which might require counter-terms outside the Hamiltonian formalism, but they can be cancelled by a redefinition of the Yang-mills electric field. The BRST identities do not fix the renormalization constants uniquely. We are free to make some choices (Andraši et al., 2009).

Solutions of coupled BPS equations for two-family Calogero and matrix models

The large N, two-family Calogero and matrix model in the Hamiltonian, collective-field approach has been studied. The Bogomol'nyi limit appears and the solutions to the coupled Bogomol'nyi-Prasad Sommerfeld equations are given by the static soliton configurations. One-parameter solutions in the strong-weak dual case have been constructed. Full classification of these solutions was presented (Bardek et al., 2009).

Deformed oscillator algebras and QFT in kappa-Minkowski spacetime

The deformed statistics and oscillator algebras of quantum fields defined in kappa-Minkowski spacetime were studied. The notion of a fully covariant flip operator was proposed and expressed to the first order in terms of the Poincaré generators alone. The R-matrices for the twisted and the covariant flip operators are compared up to first order and shown to be different. This is used to construct a new large class of deformed algebras of creation and annihilation operators (Govindarajan et al., 2009).

Homolumo gap from dynamical energy levels

A dynamical matrix model where the matrix is interpreted as a Hamiltonian representing interaction of a bosonic system with a single fermion was introduced. It was shown how a system of second-quantized fermions influences the ground state of the whole system by producing a gap between the highest eigenvalue of the occupied single-fermion states and the lowest eigenvalue of the unoccupied single-fermion states. The development of the gap in both the strong and weak coupling regimes was described (Andrić et al., 2009).

Chemical versus van der Waals Interaction in adsorption of large molecules on surfaces

Density Functional Theory as a tool of choice in modern electronic structure calculations has a deficiency in that it does not include the long range (van der Waals) interaction in the standard formulation with local or semilocal functionals. A recently proposed nonlocal functional has been im-

plemented and tests were made on benchmark examples of three aromatic molecules on Cu(110) surface. Benzene contains delocalized pi-electrons in the carbon ring, which is believed to be responsible for large amount of nonlocal interaction. In order to test that, one and two carbon atoms in the benzene molecule have been substituted with nitrogen atoms. Very interesting results obtained show that the molecules are bonded to the surface via a mixture of chemical and vdW type bonding. In one case the interpretation is that the chemical bonding to the surface is vdW triggered, i.e. the vdW interaction brings the molecule close to the surface and only then chemical bonding (charge transfer) takes place. These pioneering results have already attracted lots of attention from the scientific community (Atodiresei et al., 2009).

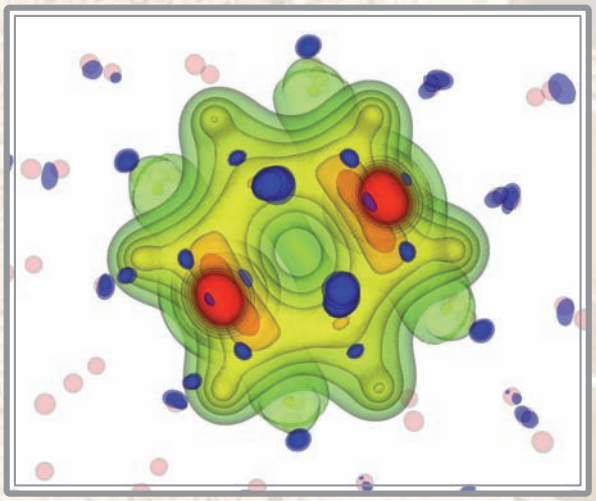


Figure 1. The nonlocal correlation binding energy density of an aromatic molecule on a metal surface, obtained using the nonlocal density functional vdW-DF

Dirac fermions in graphene on Ir(111) revealed in photoemission

Graphene, the two-dimensional honeycomb structure of carbon atoms, has attracted a lot of attention recently, both as a unique two-dimensional system and as a candidate material for future nanometer scale electronics. STM images of the graphene monolayer on Ir(111) surface show excellent alignment with the substrate and a Moiré pattern due to the small difference of periodicities. Our ARPES spectra and theoretical calculations confirm the weak bonding to the surface which leaves the Dirac electronic cones of graphene almost intact, while the Moiré superperiodicity leads to Dirac cone replicas and the opening of minigaps in the band structure (Pletikosić et al., 2009).

EDUCATION

In 2009, the members of the Division continued to be involved in lecturing undergraduate and graduate courses at the University of Zagreb, mostly at the Faculty of Science. Three students completed their Ph. D. theses.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

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

Programs supported by the Ministry od Sciences, Education and Sports

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

Research, developmental and international projects

1. QCD sum rules for exclusive decays of heavy hadrons, Blaženka Melić (International Research Project promoted by the Alexander von Humboldt Foundation, with principal investigators from RBI and University of Siegen, Germany)
2. Final state interaction in non-leptonic D- and B-decays, Blaženka Melić (Croatian-French Project in the program "COGITO" - partnership Hubert Curien)
3. Tools and Precision Calculations for Physics Discoveries at Colliders, Josip Trampetić (collaboration to the FP 6 EU RTN Network HEPTOOLS, no. MRTN-CT-2006-035505)

SELECTED INVITED LECTURES

1. Škoda Z. Higher nonabelian cohomology, Topology seminar, Ecole Politechnique Federale de Lausanne, Lausanne, Switzerland, March 8-10, 2009.

SELECTED ORGANIZED CONFERENCES

1. 4rd Croatian-Hungarian-Austrian Meeting – Non Abelian Theories, Hot Matter and Cosmology, Rab, Croatia, August 30 – September 4, 2009, organized by Anđelka Andraši and Ivan Dadić
2. 2nd School and Workshop on Quantum Gravity and Quantum Geometry, Corfu, Greece, September 13-20, 2009, Larisa Jonke, member of the organizing committee
3. International Workshop "Progress and Challenges in Flavour Physics", Primošten, Croatia, September 29 – October 4, 2009, Blaženka Melić – chairman, Kornelija Passek-Kumerički and Goran Duplančić - members of the organizing committee

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1. Andraši A, Taylor J C: Renormalization of Hamiltonian QCD. *Annals of Phys* **324** (2009), 2179.
2. Andrić I, Jonke L, Jurman D, Nielsen H B: Homolumo gap from dynamical energy levels. *Phys Rev D* **80** (2009), 107701.
3. Atodiresei N, Caciuc V, Lazić P, Blügel S: Chemical versus van der Waals Interaction: The Role of the Heteroatom in the Flat Absorption of Aromatic Molecules C_6H_6, C_5NH_5, and $C_4N_2H_4$ on the Cu(110) Surface. *Phys Rev Lett* **102** (2009), 136809.
4. Bardek V, Meljanac S, Meljanac D: Solutions of coupled BPS equations for two-family Calogero and matrix models. *Phys Rev D* **80** (2009), 1550.
5. Bilić N, Tuper G B, Viollier R D: Cosmological tachyon condensation. *Phys Rev D* **80** (2009), 023515.
6. Eilam G, Melić, B, Trampetić J: CP violation and the 4th generation. *Phys Rev D* **80** (2009), 116003.
7. Govindarajan, T R, Gupta, K S, Harikumar E, Meljanac S, Meljanac D: Deformed oscillator algebras and QFT in kappa-Minkowski spacetime. *Phys Rev D* **80** (2009), 025014-1.
8. Pletikosić I, Kralj M, Pervan P, Brako R, Coraux J, N'Diaye A T, Busse C, Michely T: Dirac Cones and Minigaps for Graphene on Ir(111). *Phys Rev Lett* **102** (2009), 056808.
9. Štefančić H: The solution of the cosmological constant problem from the inhomogeneous equation of state: A hint from modified gravity? *Phys Lett B* **670** (2009), 246.

Division of Experimental Physics

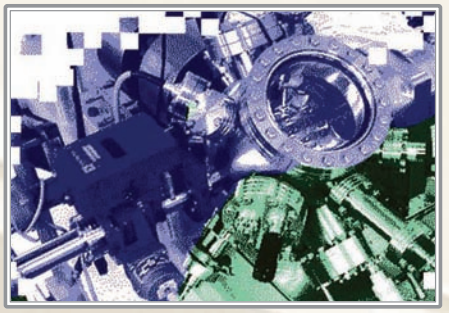
http://www.irb.hr/en/str/zef

DIVISIONAL ORGANIZATION

Head: Tome Antičić

The Division of Experimental Physics (ZEF) 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
- Nuclear analytical laboratory, Jasmina Obhođaš
- Group for hadronic spectroscopy, Alfred Švarc



OVERVIEW OF THE DIVISION

The Division of Experimental Physics is focused on experimental and theoretical nuclear and particle physics, astrophysics, and more recently in quantum information. There are over 60 staff, including more than 30 PhDs. They are involved in numerous experiments and experimental complexes abroad and in Croatia, and maintain 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-MZOŠ sources, which was used to significantly enhance its experimental capabilities.

TOP ACHIEVEMENTS

Coincident scattering for 3D profiling of light elements

A sensitive depth profiling technique has been developed on the basis of elastic scattering of MeV ions in transmission geometry. By coincident detection of both scattered and recoiled ions and by the use of scanning ion microbeam a method for 3D imaging of light elements such as carbon and oxygen has been developed (Bogdanović Radović et al., 2009).

The 'RBI-AF' FP6 project fully implemented

The FP6 project 'Rudjer Bošković Institute Accelerator Facility' was closed in November 2009 after 32 months of implementation. The project helped to stabilise and reinforce the existing research potentials of the RBI

Tandem Accelerator Facility by supporting: (i) upgrade of measurement capabilities (in-air end station, ion microprobe, material-modification-dual-beam end station; (ii) upgrade of the 6MV tandem accelerator system (its vacuum system and sputtering ion source – Figure 1); (iii) preparation of promotion brochures, organization of the workshop for targeted user-groups and upgrade of the facility web site.

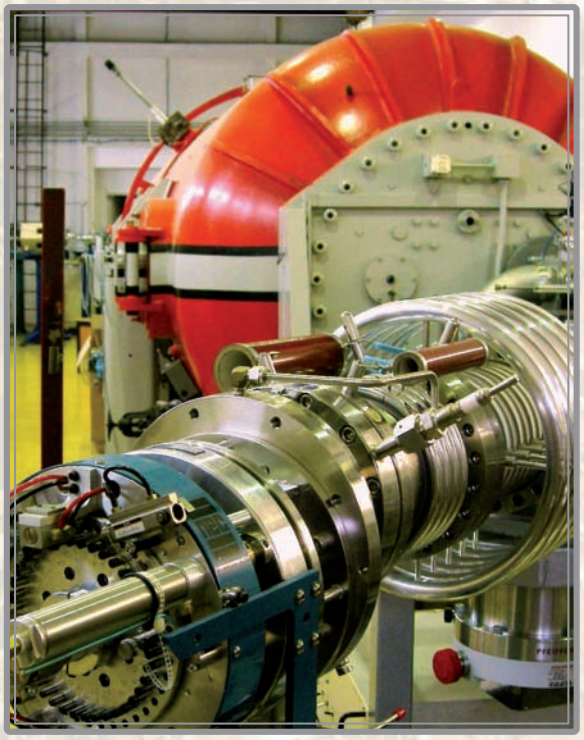


Figure 1. Sputtering ion source at the EN Tandem accelerator.

FP7 project SPIRIT started

Within the framework of the Integrated Infrastructure Initiative (I3), a new FP7 project SPIRIT started in March 2009. The SPIRIT (Support of Public and Industrial Research using Ion beam Technology) consortium integrates 11 leading European ion beam facilities from 6 EU member states, Switzerland and Croatia. Ions in an energy range from 10 keV to 100 MeV are made available for the modification and analysis of solid surfaces, interfaces, thin films and nanostructured systems. The main application areas are materials, biomedical and environmental research and technology. RBI participates in Joint Research Activities such as targeted single ion implantation for irradiation of living cells; ion-beam based analysis with ultrahigh depth resolution; ion-based 3-D tomography, and chemical and molecular imaging.

Strangeness production at threshold

In order to study the density dependence of the kaon-nucleon (*KN*) potential in details, an understanding of the strangeness production cross sections at threshold and at finite baryonic densities is essential. In order to estimate the strength of the potential, the FOPI measurements of negative pions on various targets have been compared to the results of the hadron-string-dynamics (HSD) transport-model calculations. The version of the model that includes a 20 MeV K^0N potential at the saturation density (dashed line, Figure 2) reproduces qualitatively the observed pion on Pb and carbon K^0 production yield ratio and its suppression on heavy targets at low mo-

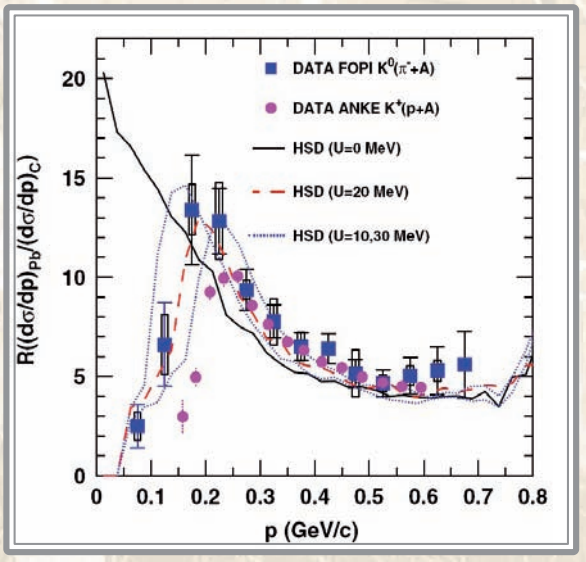


Figure 2. The ratio of K^0 yields produced by 1.15 GeV/c pions on heavy (Pb) and light (C) targets plotted as a function of the momentum p in the lab system. The full squares depict the yield ratio in this experiment. The results of the HSD model with different strengths of the KN potential are depicted by solid (black), dashed (red), and dotted (blue) lines.

menta. This observation can be explained by a repulsive K^0N potential in the nuclear medium, which accelerates kaons before they escape the nucleus (Benabderrahmane et al., 2009).

Lifetimes of N=30 exotic nuclei

The gamma sphere CLARA coupled to the magnetic spectrometer PRISMA allowed the determination of lifetimes of the first excited states of the N=30 isotones ^{50}Ca and ^{51}Sc by using a Recoil-Distance-Doppler-Shift method. The low-lying states were populated via a transfer process in the ^{48}Ca+^{208}Pb reaction. Measurement confronted to shell-model calculations indicates an orbital dependence of the core polarization along the fp shell (Valiente-Dobon et al., 2009).

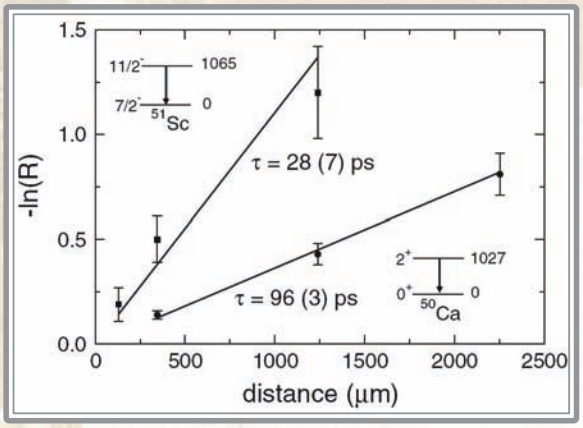


Figure 3. Negative logarithm of the experimental ratio of the yields under the peak area of the indicated electromagnetic transitions emitted after and before the thick Mg degrader, for the different target-degrader distances. It shows as well the fitted lifetime of the 2^+ and the $11/2^-$ states in ^{50}Ca and ^{51}Sc.

The Crystal Ball Spectrometer and Frozen Spin Polarized Target

In 2009 the Crystal Ball Collaboration at the Mainz Microtron (MAMI) successfully finished assembly and testing of a new Frozen Spin Polarized Target. RBI scientists have significantly contributed to this achievement. In conjunction with the new upgraded MAMI C accelerator a new phase of important experiments started in 2009. This new setup will facilitate precise measurements of the anomalous magnetic moment of the Delta resonance as well as first double polarization measurements.

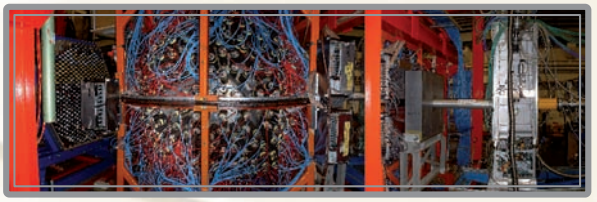


Figure 4. Panoramic view of CB and TAP Spectrometers.

Search for hadronic axions

At CERN, a group of our scientists explored the relation between the coupling constants of pseudoscalar particles that couple to a nucleon and to two photons by using the CAST helioscope to look for 14.4 keV axions that may be emitted in the M1 nuclear transition of ^{57}Fe (Andriamonje et al., 2009).

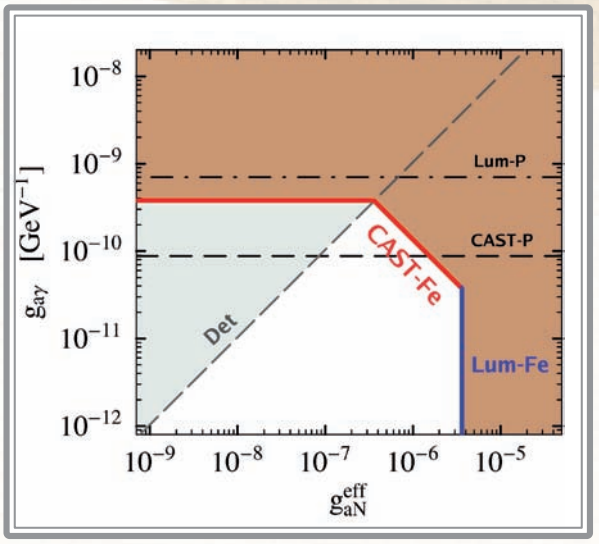


Figure 5. Results of the first implementation of axion helioscopes in search for axions emitted in nuclear de-excitations.

Search for neutrino oscillations

At LNGS, the OPERA-Zagreb group has participated in data collection and analysis of neutrino interactions in the emulsion/lead

target. That allowed checking the complete analysis chain starting from the trigger down to the neutrino vertex location in the emulsions and to the topological and kinematical characterization of the event.

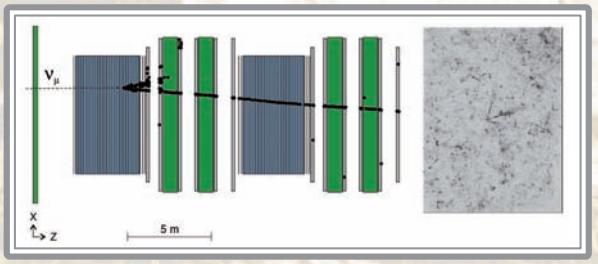


Figure 6. Neutrino interaction captured in emulsion.

Single photon detector

First prototypes of high performance single photon detector module have been built at RBI, based on a novel Si APD sensitive in VIS-NIR spectrum.

Acceleration of the Universe

It was shown that light neutrino dipole moments, as a possible source for neutrino condensates, may explain the acceleration of the universe at present (Horvat et al., 2009). The framework for an effective quantum field theory with a manifest UV/IR connection has been developed with a large number of particle species. Such a setup fills in a large gap in entropy of any non-black hole configuration of matter and the black holes, solving at the same time the multiplicity of species problem (Horvat et al., 2009). The constraint on the scale of noncommutative gauge field theory has been set using considerations of the big bang nucleosynthesis of light elements. This proves one of the strongest restrictions on the scale of noncommutativity (Horvat et al., 2009). The hadronic axions, which may be produced in the Sun by a bremsstrahlung-like process, were searched for by an axioelectric effect using the HPGe detector. A conservative upper limit on the hadronic axion mass is obtained (Kekez et al., 2009).

MAGIC Colalboration

In June 2009 the Croatian consortium (including R. Bošković Institute, University of Rijeka and University of Split) became a full member of the MAGIC (Major Atmospheric Gamma-ray Imaging Telescope) collaboration. In December the same consortium joined the CTA (Cherenkov Telescope Array) collaboration. MAGIC and CTA are large international projects in gamma-astronomy.

CMS Collaboration

The RBI group working on the Compact Muon Solenoid (CMS) Experiment at the Large Hadron Collider at CERN has continued its preparation for the first LHC collisions seen at the end of 2009. The CMS experiment has been commissioned in 2 long cosmic runs during which more than 600 million cosmic muons have been recorded, providing an optimal opportunity to test and improve the performance of the whole CMS detector, from the proper functioning of all subdetectors to the complex analysis chain allowing scientists from around the world to analyze LHC data through the LHC Computing Grid (LCG). The RBI group has been actively involved in the analysis of these cosmic data and has worked on the determination of the expected background from cosmic muons in collision data.

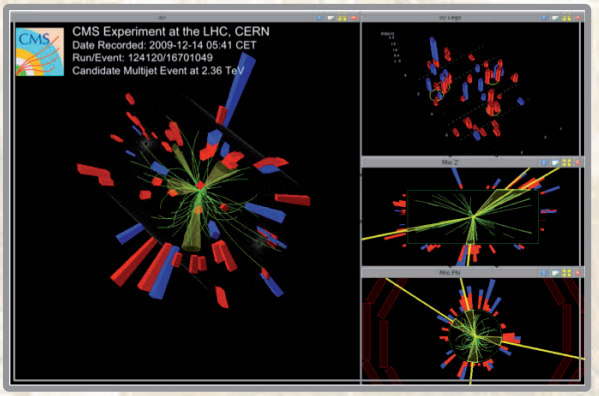


Figure 7. One of the first proton-proton collision events seen by the CMS experiment.

An analysis of the system size scan in Pb+Pb collisions at the NA49 detector at the CERN-SPS was performed at 40 A GeV and 158 A GeV to understand the crossover region of the transition from normal matter to the quark-gluon plasma phase (Alt et al., 2009).

Natural isotopes in environmental studies and radiocarbon dating

The FP7 project SOWAEUMED dedicated to the network of solid waste and water treatment between Europe and Mediterranean Countries was approved by the EU in 2009 and representatives of the Laboratory attended the kick off meeting in Barcelona.

The new system for graphite preparation of micro-sized samples for ^{14}C measurement by AMS technique was validated by participation in the VIRI intercomparison. Dating of prehistoric and mediaeval sites from Croatia and Slovenia by LSC method continued. Carbon exchange processes in atmosphere, water and lake sediments were studied together with measurements of stable isotopes (^{13}C, ^{18}O, ^{14}N) in order to asses possible anthropogenic contamination in Karst systems. Monitoring of ^{3}H activity in monthly precipitation in Croatia and Slovenia has been continued, as well as ^{14}C monitoring in biological samples and atmospheric CO_2 in the immediate vicinity of the Nuclear Power Plant Krško. The results of ^{3}H and ^{14}C activity in surface and ground waters were used for hidrogeological studies.

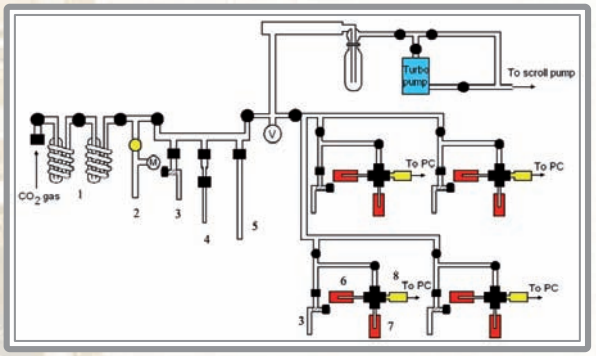


Figure 8. Vacuum line for graphite preparation of micro-samples for AMS ^{14}C dating.

Development of a unified method for the QCD compatible resonance signal extraction

The interrelation of experimentally observed nucleon resonances with theoretical QCD predictions have been studied within the scope of coupled channel, unitary and fully analytical model developed in Zagreb on the basis of traditional Carnegie-Melon-Berkeley approach. In order to avoid comparison with the notoriously model dependent Breit-Wigner parameters, a flexible set of codes has been used to extract a set of model-independent pole parameters from the world collection of partial-wave amplitudes.

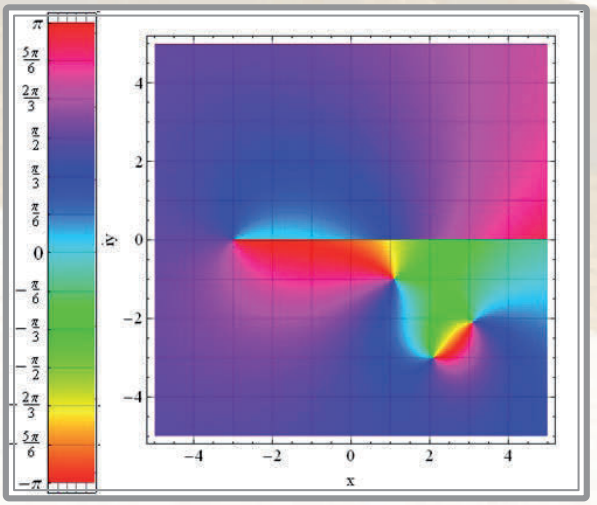


Figure 9. Resonant poles, a simple zero and a branch cut are visible on this color phase plot of the test case scattering amplitude.

Atlas of Croatian Adriatic Coastal Sea Sediments

The Atlas establishes geochemical reference baseline data for 16 chemical elements in surface sediments of the eastern Adriatic Sea and can be used for environmental and other applications. This will be of great interest to the scientific community in the field of environmental protection as well as to local, regional and international authorities leveraging sustainable development policies and capabilities based on scientific data.

NEW EQUIPMENT

Diamond as ToF start and beam-counting detector

For the new time-of-flight (ToF) barrel made of Resistive-Plate-Chambers (RPC) for the FOPI-Collaboration detector at GSI, Darmstadt a new beam detector based on a polycrystalline-CVD diamond was developed. It combines the role of a beam monitoring device and a ToF start detector. With a diamond of the surface size 2×2cm^2 and energetic heavy-ion beams (e.g. Ni of energy of 1.9*A* GeV) a time resolution better than 50 ps was obtained (Kiš et al,. 2009).

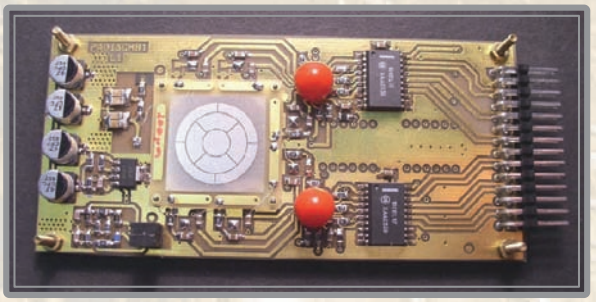


Figure 10. The p-CVD diamond with the clearly visible Al-electrode layout mounted together with the readout electronics on a PCB board which is to be operated in vacuum.

PXIe setup

Recently, The Laboratory for Hadronic physics has acquired a modular PXIe setup for precise measurements of the polarization signal from Frozen Spin Polarized Target. The setup consists of a Vector Signal Generator, Vector Signal Analyzer, and the Multifunction I/O data acquisition board. The Vector signal generator/analyzer supports generation/analysis of signals up to 6.6 GHz and will be used to simulate and analyze polarization of the target by use of nuclear magnetic resonance (NMR) technique.

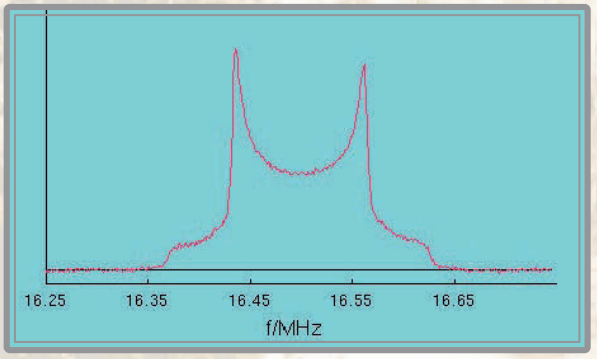


Figure 11. NMR signal of D-butanol.

Portable fast neutron generator

A portable fast neutron generator ING-27 produced by the All-Russian research Institute of Automatics (VNIIA) has been acquired for development of neutron sensor to be implemented in UNCOSS underwater vehicle.

EDUCATION

In 2009, members of the Division continued to be involved in seven courses at the University of Zagreb, mostly at the Faculty of Science. Three students completed their diplomas (graduation).

AWARDS

Promotion of scientific Excellence, Award of Croatian ministry of science, education and sport for FP7-SEC-2007-1 - UNCOSS “underwater coastal sea surveyor” project.

Promotion of scientific excellence, Award of Croatian ministry of science, education and sport for FP7-REGPOT- Clustering phenomena in nuclear physics: strengthening of the Zagreb - Catania - Birmingham partnership (CLUNA) project.

Promotion of scientific excellence, award of Croatian ministry of science, education and sport for FP7-REGPOT- Advanced Workshop for New Detectors and Electronics at the Rudjer Boskovic Institute (WONDER) project.

PATENTS

1. P20040382, Stipčević M, Quantum random number generator

Projects supported by the Ministry of Science, Education and Sports

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

Programs supported by the Ministry of Science, Education and Sports

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

Research, development and international projects

1. CLUustering phenomeNA in nuclear physics: strengthening of the Zagreb - Catania – Birmingham partnership (CLUNA), Neven Soić (FP7-REGPOT-2007-3 International Cooperation - Coordination and Support action, project number 203200)
2. Support of Public and Industrial Research using Ion beam Technology (SPIRIT), Milko Jakšić (EU FP7 project No. 227012)
3. European Risposte against Illicit tr@ffiCking (ERITRAC), Davorin Sudac, (Directorate - General Justice, Freedom And Security - Directorate D: Internal Security And Criminal Justice, “Prevention of and Fight Against Crime”
4. Underwater Costal Sea Surveyor (UNCOSS), Jasmina Obhođaš (EU FP7-SEC-2007-1, Contract No. 218148 (2008-)
5. SOWAEUMED - Network in Solid Wast and Water Treatment between Europe and Mediterranean Countries, Bogomil Obelić (European project No. 245843, call FP7-REGPOT-2009-2)
6. Development of frozen spin polarized target for Crystal Ball Collaboration at MAMI, Ivan Supek (University of Mainz for EU program I3HP TNA Contract)
7. Upgrade of the RBI Tandem Accelerator Facility (RBI-AF), Stjepko Fazinić (EC FP6 program INCO Contract 043630)
8. Isotope methods for management of drinking water resources in water scarcity areas, Nada Horvatinčić (IAEA regional project RER/8/012)
9. Global Network of Isotopes in Precipitation (GNIP) and Water Isotope System for Data Analysis, Visualisation and Retrieval (WISER), Bogomil Obelić (IAEA/WMO project)
10. Hadron Physics 2, Roman Čaplar, Ivan Supek, Alfred Švarc (EC FP 7 programme contract 227431)
11. Strengthening sustainability of nuclear research and development institutes in the modern science and technology environment, Stjepko Fazinić (National Coordinator, IAEA regional project RER/0/031)
12. Upgrading nuclear analysis techniques for air pollution monitoring, Ivančica Bogdanović Radović, (IAEA Technical Cooperation project CRO8008)
13. Measurements of differential cross sections for elastic scattering of ^{1}H and ^{4}He ions from

selected light elements, Ivančica Bogdanović Radović (IAEA Research Contract 13269)
14. Improvements of ERDA techniques using TOF spectrometer, Zdravko Siketić (IAEA Research Contract 14580)
15. Research, development and construction of portable micro X-Ray Fluorescence device, Vladan Desnica (UKF Cooperability program 1A)
16. IBIC investigation of photovoltaic cells and radiation detectors, Milko Jakšić (bilateral project with Italy)
17. Ion beam modification and characterization of nanostructured materials, Milko Jakšić (bilateral project with Serbia)
18. 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)
19. Correlations in nuclei: nucleon pairs and clusters, Suzana Szilner (Bilateral Croatian-French project within the "Cogito" programme with Hubert Curien Institute, Strasbourg)
20. OPERA collaboration, Ante Ljubičić (International collaboration between RBI , CERN (Switzerland) and LNGS (Gran Sasso, Italy))
21. CERN Axion Solar Telescope (CAST) experiment, Milica Krčmar (International collaboration between RBI and CERN, Switzerland)
22. Photon detector, Mario Stipčević (HITRA science & technology project)
23. Isotopic composition of precipitation on the region of Croatia and Slovenia, Ines Krajcar Bronić (bilateral project with Slovenia)
24. Excitation and decay of baryon resonances in a meson-theoretical approach, Alfred Švarc, (DAAD-MZOŠ bilateral cooperation agreement between Forschungszentrum Julich and RBI)
25. Precise Measurement of the $\Pi^+ \to e^+\nu$ Branching Ratio, Ivan Supek (International Collaboration between RBI and University of Virginia, Charlottesville, USA)
26. ALICE experiment, Tome Antičić (International collaboration between RBI and CERN, Switzerland)
27. NA61 experiment, Tatjana Šuša (International collaboration between RBI and CERN, Switzerland)
28. CMS experiment, Krešo Kadija (International collaboration between RBI and CERN, Switzerland)
29. Pierre Auger Observatory, Krešo Kadija, associate membership through University of Nova Gorica, Slovenia

SELECTED INVITED LECTURES

1. Jakšić M. Modern ion-beam techniques for material science and for preserving cultural heritage, European Nuclear Physics Conference, Bochum, Geramany, March 16 – 20, 2009.
2. Basrak Z. In-medium N-N cross section below 100A MeV determined from the early dynamical reaction phase, 6th International Workshop on Multifragmentation and Related Topics - IWM2009, Catania, Italy, November 4 - 7, 2009.
3. Szilner S. Quasi-elastic reactions: a survey on recent results, 18th International School on Nuclear Physics, Neutron Physics and Applications, Varna, Bulgaria, September 21-27, 2009.
4. Szilner S. Quasi-elastic reactions: a survey on recent results, International Symposium on Exotic Nuclei - EXON09, Sochi, Russia, 28th September - 2nd October 2009.
5. Zorić M. Energy and isospin dependence of elliptic flow – An alternative analysis of the LAND-FOPI data, ESF Exploratory Workshop on How to Constrain the High Density Symmetry Energy, Zagreb, Croatia, October 16 - 18, 2009.
6. Jakovčić K (for the CAST collaboration). Search for monoenergetic solar axions with the CAST experiment. 5th Patras Workshop on Axions, WIMPs and WISPs, Durham, UK, July 13 - 17, 2009.
7. Švarc A. Poles of PWD and PW amplitudes, Polarization Observables and Partial Wave Analysis, March 1 - 4 , Bad Honnef, 2009.
8. Švarc A. Bare and Dressed Poles of PW Data and PW Amplitudes, The 5th International Pion Nucleon PWA Workshop and Interpretation of Baryon Resonances, ECT*, Trento, Italy , June 1 – 5, 2009.
9. Ceci S. Resonance Parameter Extraction, The 5th International Pion Nucleon PWA Workshop

and Interpretation of Baryon Resonances, ECT*, Trento, Italy , June 1 – 5, 2009.
10. Zauner B. Problems with Nucleon Resonances, The 5th International Pion Nucleon PWA Workshop and Interpretation of Baryon Resonances, ECT*, Trento, Italy , June 1 – 5, 2009.
11. Švarc A. Inherent model dependence of Breit-Wigner parameters, poles as a true signal of resonance properties. The Jefferson Laboratory Upgrade to 12GeV (INT 09-3), November 7 – 16, 2009.
12. Švarc A. Continuum ambiguities as a limitation factor in single-channel PW analysis. The Jefferson Laboratory Upgrade to 12GeV (INT 09-3), November 7 – 16, 2009.
13. Valković V, Obhođaš J, Sudac D. Environmental Security of the Coastal Sea Floor. "2009 Winter Meeting of the American Nuclear Society (ANS) - Highlights of AccApp'09", Washington, USA, November 15-19, 2009.

SELECTED ORGANIZED CONFERENCES

The international nuclear physics conference ''Nuclear Structure and Dynamics'' organized by the RBI Laboratory for Nuclear Physics and the University of Zagreb and co-chaired by S. Szilner was held from 4th to 8th May 2009 in Dubrovnik. At this large international conference open questions and challenges of the contemporary nuclear structure and dynamics have been reviewed.

The 14th "Collaboration Meeting of the Compressed Baryonic Matter Experiment at FAIR" organized by the RBI Laboratory for Nuclear Physics and the University of Split and co-chaired by R. Čaplar was held from 6th to 9th October 2009 in Trogir. This large international meeting was devoted to the physics of strongly compressed nuclear matter and to the progress achieved in the development of new and advanced detectors needed for the high interaction-rate experiments planned at FAIR.

The Exploratory Workshop on ''How to Constrain the High Density Symmetry Energy'' sponsored by European Science Foundation and organized by the RBI Laboratory for Nuclear Physics by Zoran Basrak was held from 16th to 18th October 2009 in Zagreb. It was devoted to the isospin-dependent component of the nuclear equation-of-state which has a crucial impact on physics of compact stars and supernova dynamics.

SELECTED PUBLICATIONS

1. Bogdanović Radović I, Jakšić M, Schiettekatte F: Technique for sensitive carbon depth profiling in thin samples using C–C elastic scattering. *J Anal At Spectrom* **24** (2009), 194.
2. Mandić L, Fazinić S, Jakšić M: Chemical effects on the $K\beta_{2,5}$ and Kβ'' x-ray lines of titanium and its compounds. *Phys Rev A* **80** (2009), 042519.
3. Benabderrahmane ML (FOPI Collaboration - RBI: Basrak Z, Čaplar R, Gašparić I, Kiš M, Korolija M): Measurement of the In-Medium K0 Inclusive Cross Section in π--Induced Reactions at 1.15 GeV/c. *Phys Rev Lett* **102** (2009), 182501.
4. Corradi L, Pollarolo G, Szilner S: Multinucleon transfer processes in heavy-ion reactions. *J Phys G – Nucl & Part Phys* **36** (2009), 113101-1-43 (review paper).
5. Stefanini A (PRISMA Collaboration - RBI: Szilner S): How does fusion hindrance show up in medium-light systems? The case of $^{48}Ca + ^{48}Ca$. *Phys Lett B* **679** (2009), 95.
6. Krambrich D (Crystal Ball Collabopration - IRB: Knežević A, Korolija M, Mekterović D, Supek I): Beam-Helicity Asymmetries in Double Pion Photoproduction off the Proton. *Phys Rev Lett* **103** (2009), 052002.
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13. Andriamonje S (CAST collaboration - RBI: Jakovčić K, Krčmar M, Lakić B, Ljubičić A): Search for 14.4 keV solar axions emitted in the M1-transition of {57}^Fe nuclei with CAST. *J Cosmol Astropart Phys* **12** (2009), 002.
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Division of Materials Physics

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

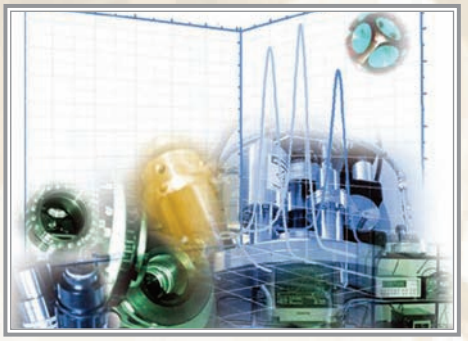
ZFM

DIVISIONAL ORGANIZATION

Head: Nikola Radić

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

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



OVERVIEW OF THE DIVISION

The Division of Materials Physics is focused on fundamental and applied studies of physical parameters and processes which describe and connect the microscopic, mesoscopic and macroscopic properties of condensed matter and molecules. Nanoscience and nanotechnology has been the most active direction of both fundamental scientific research and developments in technology. Fundamental research in the field of molecular and solid state physics placed special emphasis on vibrational spectroscopy of a wide range of systems. Strongly nonlinear effects in laser-matter interaction and self-organization in condensed systems continue to be subjects of intensive research. The Division has about 30 staff members, about a quarter of which are PhD students. The results of research by members of the Division during 2009 have been published in 40 papers in journals listed in Current Contents, with an average impact factor per paper of 1.98.

TOP ACHIEVEMENTS

Formation of three-dimensional quantum dot superlattices in amorphous dielectric matrix

Quantum dots ordered in regular lattices, called quantum dot superlattices, offer numerous possibilities for the creation of novel materials. The formation of such structures during multilayer deposition has been studied and explained satisfactorily only in crystalline materials. Here we report the spontaneous formation of quantum dot superlattices in amorphous systems. The observed superlattices comprise Ge quantum dots embedded in amorphous SiO_2 matrix. The internal structure and shape of Ge quantum dots can be controlled by post-deposition thermal annealing.

The superlattices show collective behavior properties that appear to be the consequence of a regular ordering of quantum dots. The observed self-organized growth is explained

and successfully simulated by a theoretical model based on the interplay of diffusion-mediated nucleation and surface morphology effects. The presented results can be applied more generally and show the ability of formation of regularly ordered, densely packed and uniformly-sized quantum-dot arrays in amorphous matrices (Buljan et al., 2009).

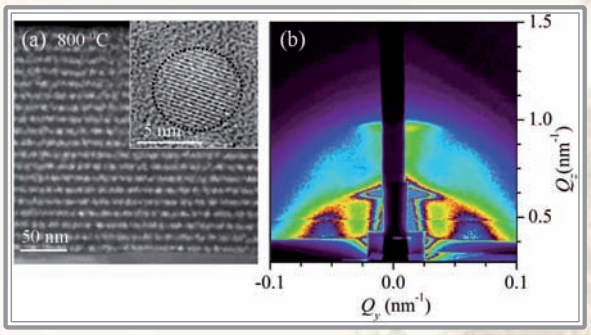


Figure 1. (a) TEM image, the corresponding HR-TEM image of typical QD (inset), and (b) GISAXS intensity map of the film annealed at T_a = 800 ^{0}C. The ordering of the dot positions in a QD superlattice causes appearing of intense diffraction (Bragg) spots in the GISAXS map.

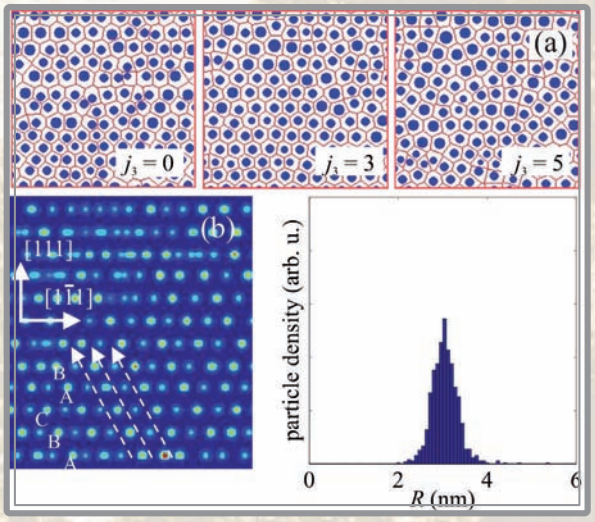


Figure 2. Results of the Monte-Carlo simulations of the dot growth. (a) Positions and sizes of the dots on the substrate surface j_3 = 0, and on the interfaces j_3 = 3, 5. The diameter of the circles represents the size of a particular dot; the lines denote the Voronoi polygons, from which the adatoms are attracted to a growing dot. (b) Simulated cross-section of a QD multilayer, the growth direction corresponds to the [111] direction in the dot lattice. The ABCABC spacing is indicated. (c) Histogram of the dot sizes in the multilayer. In the simulation, the inheritance factor C = 0.75 was assumed

Identification of hydrogen bond modes in polarized Raman spectra of single crystals of α-oxalic acid dihydrate

Oxalic acid dihydrate was investigated by polarized Raman spectroscopy both in protonated and deuterated forms. It was found that hydrogen bonding is strongly anharmonic, with ν(OH) and ν(OD) falling in the same interval 1850 – 1900 cm^{-1}, which suggests that the potential governing the proton dynamics is of the asymmetric double-minimum type with a very low barrier. The calculated normal coordinates show a strong participation of the bending modes of water molecules in almost all internal acid motions, as well as in the external phonons (Mohaček Grošev et al., 2009).

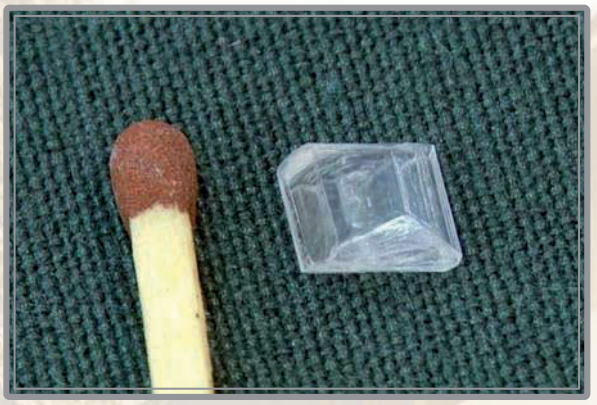


Figure 3(a). Monocrystal of protonated oxalic acid dihydrate, space group $P2_1/n$, compared to a match. Crystal b axis points along the long side of the match.

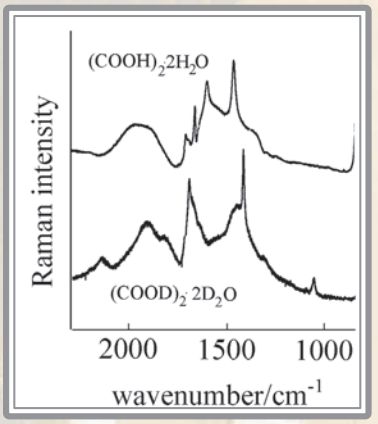


Figure 3(b). Comparison of Raman spectra for protonated (upper) and deuterated (lower) oxalic acid dihydrate for y(zz)x monocrystal orientation.

Optical spectroscopy study of nc-Si-based p–i–n solar cells

Amorphous-nano-crystalline silicon (a-nc-Si) based p-i-n thin film structures were produced by RFPECVD method with various individual crystal sizes, size distributions and crystal fraction. A comparison between structural properties inferred by Raman spectroscopy and spectral distribution of dielectric function (Figure 4) confirmed a strong connection between optical and crystalline properties of a-nc-Si films which open the possibility of tailoring the optical behavior of the films that can be used for design of third-generation photovoltaic devices (Sancho-Parramon et al., 2009).

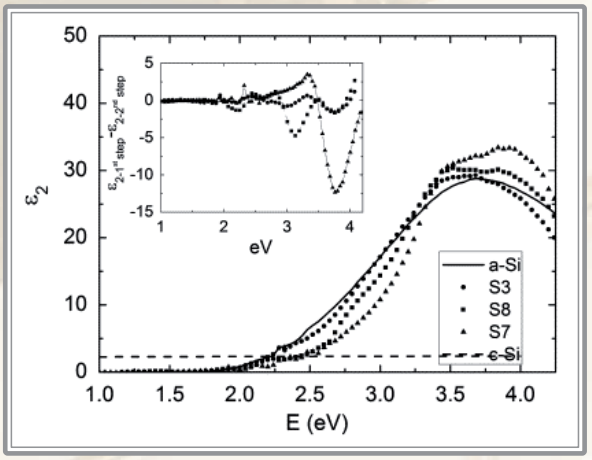


Figure 4. Spectral distribution of the imaginary part of the dielectric function of a-nc-Si films with various crystalline fractions. Inset shows difference between dielectric function obtained by direct data inversion and using the Tauc-Lorentz model.

Nanostructuring of a silicon surface by laser redeposition of Si vapor

The patterns of Si nanoparticles on Si-wafer have been formed by means of an IR laser using the redeposition of Si-vapor method in the experimental configuration which does not allow free vapor expansion. The configuration, called «semiconfined», which directs the Si-vapor expansion into well defined micro-channel, has been used. By using small laser power density (below the ablation threshold), it was shown that the process of surface nanostructuring can be controlled.

(i) The Si surface low density nanostructuring (shown in Figure 5a) may be used for development of structures which make possible anchoring (pinning) of various filaments including polymers, biopolymers, or even DNA molecules.

(ii) The Si surface high density nanostructuring (shown in Figure 5b) may be used for development of various types of sensors.

The formation of low and high density nanostructuring has been theoretically described on the basis of a unique model of Si-vapor-turbulence in the microchannel (Lugomer et al., 2009).

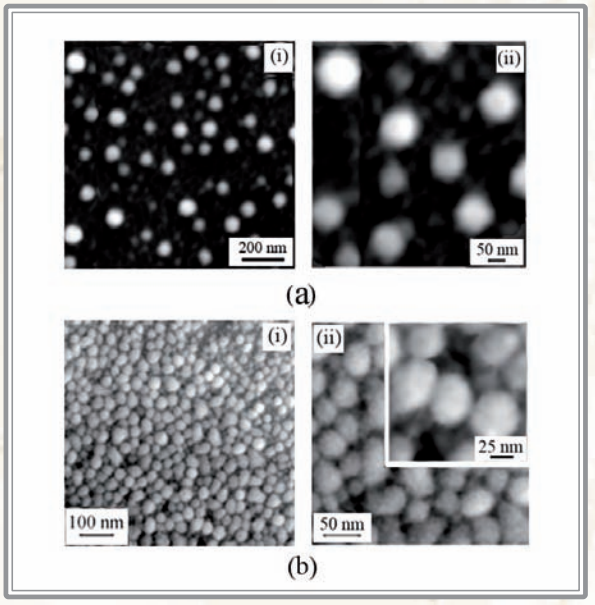


Figure 5. (a) The Si surface low density nanostructuring by laser redeposition of Si vapor. (b) The Si surface high density nanostructuring by laser redeposition of Si vapor.

EDUCATION

Members of the Division of Materials Physics teach 11 graduate and 3 postgraduate courses of physics and related topics at the Faculty of Sciences, Faculty of Electrical Engineering and Computing, Faculty of Chemical Engineering and Technology in Zagreb and elsewhere.

SELECTED INVITED EDUCATIONAL COURSE FOR INDUSTRY

In addition to the established lecturing in postgraduate courses at the Faculty of Science of the University of Zagreb, a specialized educational course to fellows in the pharmaceutical industry was held:

Biserka Gržeta, Jasminka Popović. X-ray diffraction of polycrystalline sample as an analytical method in industry: Educational course for industry, Pliva d.d., Zagreb, Croatia, 7-14 December 2009.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

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

Program supported by the Ministry of Science, Education and Sports

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

Research, developmental and international projects

1. Study of defects in semiconductors irradiated by fast neutrons, Branko Pivac (Croatian-Slovenian bilateral project 2009-2010)
2. Influence of quantum confinement on vibrational properties in nanocrystalline silicon, Davor Gracin (Croatian-Slovenian bilateral project)
3. Nanocrystalline silicon as a possible candidate for “third generation” of solar cells, Davor Gracin (Croatian-Slovenian bilateral project)
4. Preparation of surfaces with special properties by ion impalantation and laser interactions, Stjepan Lugomer (Croatian-Hungarian bilateral project)
5. Atom probe tomography and electrical characterization of doping in Germanium, Ivana Capan (COGITO Croatian-French bilateral project 2009-2010)
6. Study of oxygen precipitation and structural defects in single crystal silicon, Branko Pivac (Croatian - Chinese Scientific and Technological Cooperation)
7. Silicon nanocrystals solar cells ... Properties and characterization, Ivana Capan (Unity Through Knowledge Fund – Young Researchers Program; 01.10.2009 - 30.09.2011)
8. The origin of structural defects in silicate glasses and their effects upon the properties, Davor Gracin (National Science Foundation of Croatia)

SELECTED PUBLICATIONS

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2. Djerdj I, Cao M, Rocquefelte X, Černý R, Jagličić Z, Arčon D, Potočnik A, Gozzo F, Fabia M, Niederberger M: Structural Characterization of a Nanocrystalline Inorganic-Organic Hybrid with Fiber-Like Morphology and One-Dimensional Antiferromagnetic Properties. *Chem Mater* **21** (2009), 3356.

3. Buljan M, Bogdanović-Radović I, Karlušić M, Desnica U V, Dražić G, Radić N, Dubček P, Salamon K, Bernstorff S, Holý V: Formation of long-range ordered quantum dots arrays in amorphous matrix by ion beam irradiation. *Appl Phys Lett* **95** (2009), 063104.
4. Mohaček Grošev V, Grdadolnik J, Stare J, Hadži D: Identification of hydrogen bond modes in polarized Raman spectra of alpha oxalic acid dihydrate. *J Raman Spectrosc* **40** (2009), 1605.
5. Buljan M, Desnica U V, Dražić G, Ivanda M, Radić N, Dubček P, Salamon K, Bernsdorff S, Holy V: The influence of deposition temperature on the correlation of Ge quantum dot positions in amorphous silica matrix. *Nanotechnology* **20** (2009), 085612.
6. Ivanković M, Brnardić I, Ivanković H, Huskić M, Gajović A: Preparation and properties of organic-inorganic hybrids based on poly (methyl methacrylate) and sol-gel polymerized 3-glycidyloxypropyltrimethoxysilane. *Polymer* **50** (2009), 2544.
7. Buljan M, Desnica U V, Ivanda M, Radić N, Dubček P, Dražić G, Salamon K, Bernsdorff S, Holy V: Formation of three-dimensional quantum-dot superlattices in amorphous systems: Experiments and Monte Carlo simulations. *Phys Rev B* **79** (2009), 035310.
8. Buljan M, Desnica U V, Radić N, Dražić G, Matej Z, Vales V, Holý V: Crystal structure of defect-containing semiconductor nanocrystals - an X-ray diffraction study. *J Appl Cryst* **42** (2009), 660.
9. Sancho-Parramon J, Gracin D, Modreanu M, Gajović A: Optical spectroscopy study of nc-Si-based p-i-n solar cells. *Sol Energy Mater Sol Cells* **93** (2009), 1768.
10. Buljan M, Pinto S R C, Kashtiban R J, Rolo A G, Chahboun A, Bangert U, Levitchev S, Holy V, Gomes M J M: Size and spatial homogeneity of SiGe quantum dots in amorphous silica matrix. *J Appl Phys* **106** (2009), 084319.
11. Lugomer S, Maksimović A, Karacs A, Toth L: Nanostructuring of a silicon surface by laser deposition of Si vapor. *J Appl Phys* **106** (2009), 114308.

Books

Aleksandra Turković: Raman Study of the $Ag_8W_40_{l6}$ in the Superionic System AgI + $Ag_8W_40_{l6}$, VDM Verlag, 2009, http://www.vdm-publishing.com/.

Division of Laser and Atomic Research and Development

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

DIVISIONAL ORGANIZATION

Head: Hrvoje Zorc

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

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

OVERVIEW OF THE DIVISION

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

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

TOP ACHIEVEMENTS

Optical thin films

Research on the plasmonic properties of metal island films (MIF) and their applications is ongoing. Such films show unique optical properties due to the surface plasmon resonance (SPR) of electrons in metal clusters. By varying conditions in the preparation of these films, the structural and geometrical properties of the clusters can be varied, enabling tuning of the optical properties of these films. Structural and optical characterization are carried out using different techniques (AFM, GISAXS, RBS, ellipsometry), both locally and in the framework of international cooperation. Electric field assisted dissolution (EFAD) of metal clusters, involving the instantaneous application of an electric field and increased temperature enables structuring of such films.

The width of the SPR of metal particles increases as the particle size reduces due to confinement effects that modify the metal dielectric function. In the limit of very low particle concentration, particle size can be directly related to the plasmon width. For noble metals the contribution of interparticle interaction to SPR width cannot be neglected even at volume concentrations of a few per cent (Sancho-Parramon et al., 2009). The results can be useful in extending nanoparticle sizing from optical extinction spectroscopy beyond the dilute limit required by classical Mie theory.

Application of EFAD to MIF, followed by thermal annealing, results in the formation of metal nanoparticles embedded in a glass matrix. The results suggest that the depth profile of metal particles might be tailored by modification of the parameters of metal film dissolution. Variation of thermal annealing parameters allows for control of nanoparticles size. Thus, the surface plasmon absorption intensity and line shape are changed, enabling tuning of the optical properties of the sample.

Three dimensional (3D) photonic microstructures are produced by the locally selective EFAD of metal clusters embedded in dielectric multilayer stacks (Figure 1). The produced structures show a highly tailorable optical behaviour that combines the interferential effects of multilayer stacks and the SPR of non dissolved metal clusters (Figure 2). Due to its feasibility and the possibility to widely modify the optical properties of the resulting structures, the current approach represents a promising method for the production of novel components based on 3D-metallodielectric photonic structures.

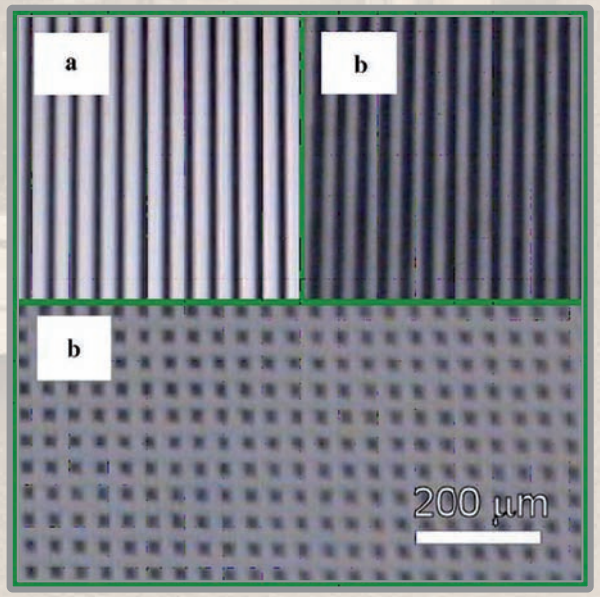


Figure 1. Optical microscopy pictures of the grating used as electrode (a), multilayer sample after EFAD process (b) and multilayer sample after two consecutive EFAD treatments, with the electrode rotated 90◦ in the second treatment (c).

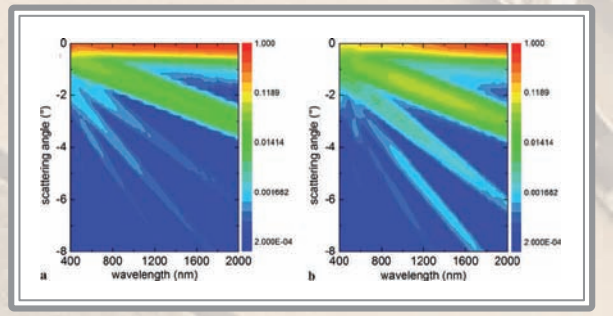


Figure 2. Wavelength-dependence of diffraction pattern of multilayer structures produced by EFAD treatment: (a) multilayer structure BK7/(Ag/SiO_2)^5 with thickness of 7 nm of Ag and 100 nm of SiO_2 and (b) multilayer structure BK7/(X/SiO_2)^5, in which X represents a multilayer of Ag and SiO_2 films

Signal processing

Research activities related to theory and innovative applications of blind and non-Gaussian information processing methods continue to be a focus for the Division. A new algorithm for unsupervised or blind decomposition of low-dimensional multi-spectral image with spectrally similar materials has been derived for robust demarcation of tumors. Using recent results from nonnegative matrix factorization theory, a method was derived for blind multi-spectral image decomposition that contains more materials than spectral bands. A new concept for blind separation of multi-dimensional signals has been derived using tensor factorization and demonstrated on blind multi-spectral image decomposition and blind image deconvolution (Kopriva, 2009). Dependent component analysis based matrix factorization has been applied to multi-frame blind image deconvolution of turbulence degraded images (Du and Kopriva, 2009). These original results will find applications in remote sensing and medical imaging.

A new research topic has been initiated in the field of chemometrics. Recent advancement in the blind source separation domain, known as sparse component analysis, has been applied to blind extraction of analytes (pure components) from a smaller number of mixtures. The concept has been demonstrated experimentally in FT-IR spectroscopy,

NMR spectroscopy (Kopriva et al., 2009) and mass spectrometry. The most recent result in this area has been the subject of a patent application with claims related to applications in natural products research and identification of biomarkers from mixtures of biological fluids and tissue extracts.

As a side issue, a new algorithm for direction finding of non-Gaussian radio emitters has been derived (Du and Kopriva, 2009).

PATENTS

1. PCT/HR2009/000028, Kopriva I, Jerić I, Method of and system for blind extraction of more pure components than mixtures in 1D and 2D NMR spectroscopy and mass spectrometry combining sparse component analysis and single component points

NEW EQUIPMENT

1. Spectroscopic ellipsometer Woollam VVASE

EDUCATION

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

AWARDS

Award to Ivica Kopriva: The Croatian State Award, the most prestigious scientific award in Croatia, was given to Ivica Kopriva, senior scientist in the Division of Laser and Atomic R&D. Ivica Kopriva was granted the award for scientific achievements in the year 2008 in the field of technical sciences.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

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

Research, developmental and international projects

1. Optical properties of metal nanoparticles embedded in dielectric multilayers, Project in collaboration with Institute of Nanostructured Materials and Photonics, Weiz, Austria (bilateral project with Austria), Zorc H.
2. Collaboration in development of optical systems for the company HS Produkt, Croatia (applied project with HS Produkt)

SELECTED INVITED LECTURES

1. Sancho-Parramon J, Janicki V, Zorc H, Lončarić M, Modification of optical properties of metal islands films by electric field assisted dissolution of clusters, 16th International Scientific Meeting on Vacuum Science and Technique, Bohinj, Slovenia, June 4-5, 2009
2. Zorc H, Spectroscopic Ellipsometer Woollam VVASE, 16th International Scientific Meeting on Vacuum Science and Technique, Bohinj, Slovenia, June 4-5, 2009
3. Kopriva I, (Semi-)blind Source Separation with Sparseness Constraints, The George Washington University, School of Engineering and Applied Science, Department of Electrical and Computer Engineering, Washington D.C., USA, February 13, 2009
4. Kopriva I, Opponent on the PhD Thesis defense of Toni Huovinen “Independent Component Analysis in DS-CDMA Multiuser Detection and Interference Cancellation,” Department of Communication Engineering, Tampere University of Technology, Tampere, Finland, January 9, 2009

SELECTED PUBLICATIONS

1. Sancho-Parramon J: Surface plasmon resonance broadening of metallic particles in the quasi-static approximation: numerical study of size confinement and interparticle interaction effects. *Nanotechnology* **20** (2009), 2357062.
2. Pivac B, Dubcek P, Capan I, Zulim I, Betti T, Zorc H, Bernstorff S: Nano Si superlattices for the next generation solar cells. *J Nanosc Techn* **9** (2009), 3853.
3. Lončarić M, Sancho-Parramon J, Pavlović M, Zorc H, Dubček P, Turković A, Bernstorff S, Jakopic G, and Haase A: Optical and structural characterization of silver islands films on glass substrates. *Vacuum* **84** (2009), 188.
4. Kopriva I, Jerić I, Smrečki V: Extraction of multiple pure component ^{1}H and ^{13}C NMR spectra from two mixtures: novel solution obtained by sparse component analysis-based blind decomposition. *Anal Chim Acta* **653** (2009), 143.
5. Kopriva I: 3D Tensor Factorization Approach to Single-frame Model-free Blind Image Deconvolution. *Opt Lett* **34** (2009), 2385.
6. Kopriva I, Cichocki A: Blind Multi-spectral Image Decomposition by 3D Nonnegative Tensor Factorization. *Opt Lett* **34** (2009), 2210.
7. Du Q, Kopriva I: Dependent component analysis for blind restoration of images degraded by turbulent atmosphere. *Neurocomputing* **72** (2009), 2682.

Division of Electronics

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

DIVISIONAL ORGANIZATION

Head: Tomislav Šmuc

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

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

OVERVIEW OF THE DIVISION

Main topics of research in the Division of electronics combines research in the fields of artificial intelligence (machine learning and intelligent data analysis methods, knowledge representations for information systems) with advanced measurement techniques and signal analysis. Emphasis is placed on tailored applications of these techniques in biomedicine, computational biology and bioinformatics, but also in engineering and economics, which is reflected in the multi-disciplinary character of our collaborations and publications record. The core of our research activities is within the long term MSES financed research programme "Computational knowledge discovery in scientific applications" lead by Dr. D. Gamberger. The programme includes three divisional projects and two projects from the University of Zagreb. In 2009 members of the Division organized a workshop around the topics covered by the programme, attended by the wider research audience and industrial partners (http://lis.irb.hr/KDSA2009/).

In addition to it's long term research projects, in 2009 the Division obtained three information technology projects (whose principal investigators are PhD students of the Division), one bilateral research project with Hungarian partners, as well as one R&D project with an industrial partner.

Senior Division members continue to contribute significantly to the graduate and postgraduate curricula of University of Zagreb through a number of graduate engineering courses and PhD courses in bioinformatics and biomedicine.

TOP ACHIEVEMENTS

Knowledge technologies and computer science

Large scale in-silico annotational experiments in genomics and proteomics

Two large scale problems are currently pursued using novel machine learning approaches: (i) determining the prevalence

of codon usage bias, related to translational process optimization, over the majority of sequenced prokaryotic genomes, and (ii) multi-label classification approach to functional annotation of genes/proteins utilizing phylogenetic profiles based on data from OMA (database of orthologous genes from sequenced prokaryotic genomes). The latter project started as a collaboration with the Department of Knowledge technologies (Josef Stefan Institute, Ljubljana), and will continue through enlarging the collaboration including the Computational Biology Group from ETH, Zurich.

Algorithms for automata representation

In computer science, finite state automata (FSA) are widely used concepts for representing finite languages, i.e. sets of strings. FSAs can be efficiently implemented and they have been used in many applications where there is a need to store and search large sets of string type data (various natural language applications, internet lookup tables, indexing large collections of data). An efficient implementation means that the automaton is compact and fast to search and construct. A standard solution is to use minimal finite state automaton.

We focus our research on a Recursive Automaton (RA), which is, regarding automata compression, a step further from the minimal automaton. We have recently demonstrated that our variant of RA is distinctly better than other similar efforts for storing a gazetteer (special dictionary of geographic data). Currently our research is directed towards finding a linear and, if possible, incremental algorithm for construction of this, most space efficient, version of RA.

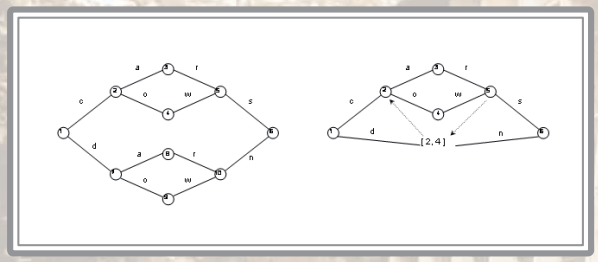


Figure 1. (a) minimal finite state automaton, and (b) recursive automaton for the same set of strings.

Knowledge representation and reasoning for healthcare

In 2009 we completed a three year long research and development term within the HEARTFAID project (EU6FP ICT-STREP). The Division has made significant contributions to the knowledge representation and decision support system of the HEARTFAID platform. The scientific contribution to the project included the coupling of Bayesian network reasoning with description logic reasoning upon the ontology of the domain of the heart failure and has resulted in a PhD thesis.

Advanced signal processing techniques and measurement systems

Time series analyses of real world data

Primary focus are the applications to human walking, jaw movement (Figure 2) and

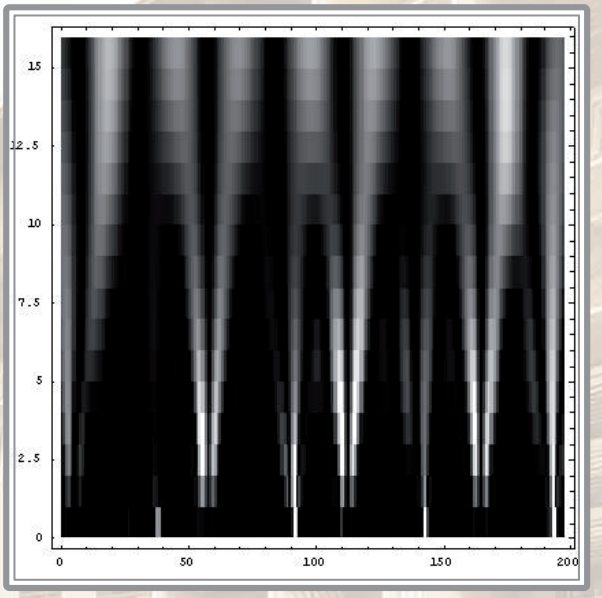


Figure 2. CWT of human jaw opening-closing cycles (head straight).

feast dynamics. Characterization of system states based on different dynamics patterns and fractal features is performed. This includes interpretation algorithms based on different dynamic parameters originating from spectral analyses and wavelet transform. Currently we are develping new fractal features extraction methods based on artificially generated fractional Gaussian noise data (fGn).

Surrogate models for measurement systems

The application of computational intelligence methods in measurement systems is aimed to decrease the complexity of the measurement systems using machine learning surrogate models for the reconstruction of true measured values. The Group Method of Data Handling (GMDH) with novel metrics for model selection is developed and implemented in software. We proposed a compound root relative squared error measure with weighting coefficient, which adjusts the GMDH models (see Figure 3 for an illustration) with respect to both the complexity and the accuracy. By combining meta-modelling with different machine learning techniques we have derived useful surrogates of complex calculation procedures. The simplified models of natural gas properties and flow correction with predefined accuracy and complexity were generated by using GMDH, Artificial Neural Networks and Support Vector Regression. The possibilities of their real-time applications are verified by simulating the measurement error and the calculation times in flow rate measurement of natural gas.

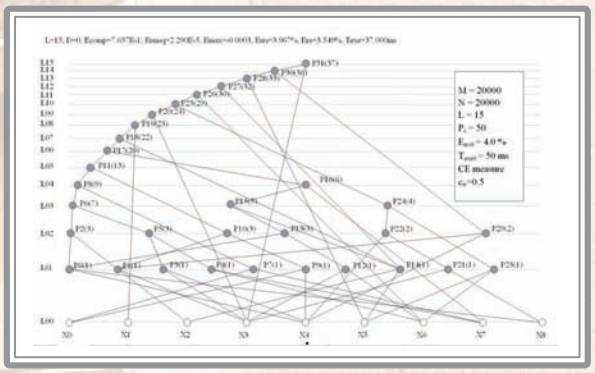


Figure 3. Polynomial graph of the best GMDH surrogate model of the flow rate correction factor.

EDUCATION

During 2009, members of the Division led 5 courses at three faculties of the University of Zagreb.

AWARDS

Branka Medved Rogina was awarded Croatian Academy of Engineering Annual Award 'Richard Podhorsky' for 2008, for distinguished scientific contribution in the development and application of high resolution timing measurement methods and testing of microelectronics and optoelectronics devices, with an emphasis on using new electronic technologies in the Republic of Croatia and beyond.

PROJECTS

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

Programs supported by the Ministry of Science, Education and Sports

1. Computational Knowledge Discovery in Scientific Applications, Dragan Gamberger

Research, developmental and international projects

1. Intelligent Data Analysis, Dragan Gamberger (Croatian-Slovenian bilateral project)

2. Reconfigurable embedded systems based assistive applications for elderly people, Branka Medved Rogina (Croatian-Hungarian intergovernmental S&T cooperation programme).
3. Reliability of Programmable Logic Devices in Industrial Embedded Systems, Branka Medved Rogina (R&D project with Končar Institute for Electrical Engineering)
4. Upgrade of the document management software, Tomislav Šmuc (R&D IRCRO project)
5. REVIGO: Web application for reduction and visualization of the set of Gene Ontology categories, Fran Supek (Information technology project, MSES)
6. GORBI (Gene Ontology at Ruđer Bošković Institute): Web application for predicting protein functional context, Nives Škunca (Information technology project, MSES)
7. GMDH for Weka, Ivan Ivek (Information technology project, MSES)

SELECTED PUBLICATIONS

1. Kralj Novak P, Lavrač N, Gamberger D, Krstačić A: Methodology for contrast set mining through subgroup discovery. *J Biomed informatics* **42** (2009), 113.
2. Rios-Morales R, Gamberger D, Šmuc T, Azuaje F: Innovative methods in assessing political risk for business internationalization. *Res Int Business Finance* **23** (2009), 144.

Division of Physical Chemistry

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

ZFK

DIVISIONAL ORGANIZATION

Head: Aleksandar Sabljić

- 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

In 2009 members of the Division published more than 50 articles in atmospheric chemistry, chemical kinetics, structural chemistry, theoretical chemistry, modelling of physical and chemical processes, structural and chemical analyses and in biosciences. A significant part was published in the highest ranking journals in their respective fields. One third of those contributions were performed within international collaborations. A large number of fruitful international collaborations demonstrated a strong presence of the Division in the European Research Area. Divisional members also contributed extensively (in about 40 courses) to undergraduate and graduate education in Croatia. Last but not least, the Divisional members organized 2 major international conferences with participation of Nobel laureates; 10th International Summer School on Biophysics and 3rd Adriatic Meeting on Computational Solutions in the Life Sciences. These highly regarded and well known series of conferences generated revenues of 155.000 US dollars and the majority of contributions was from the international sources (e.g. FP6, ESF, UNESCO, IUPAB, EBSA).

TOP ACHIEVEMENTS

Complex Aqueous Chemistry of Glycine Anion

A pulse radiolysis was carried out of the rate constants and kinetic isotope effects of hydroxyl radical induced H/D abstraction from glycine anion in water. The rate constants and yields of three predominantly formed radicals, glycyl (NH_2-·CH-CO_2-), aminomethyl (NH_2-·CH_2), and aminyl (·NH-CH_2-CO_2-), as well as of their deuterated analogs, were of a comparable magnitude. The unusual variety of products for a reaction between two small and simple species indicated a complex mechanism with several simultaneous reactions. Thus, a theo-

retical modeling of the reaction mechanism and kinetics was performed using the density functional theory with the BB1K functional (employing the polarizable continuum model for the aqueous phase), and improved canonical variational theory. A number of hydrogen-bonded prereaction complexes and transition states were detected. In particular, the calculations pointed to a significant mechanistic role of the three-electron two-orbital (σ/σ* N∴O) hemibonded complexes in the aqueous phase (Štefanić et al., 2009). Very good agreement was achieved with the measured rate constants and kinetic isotope effects after adjusting the calculated reaction barriers and NH(D) stretching frequency.

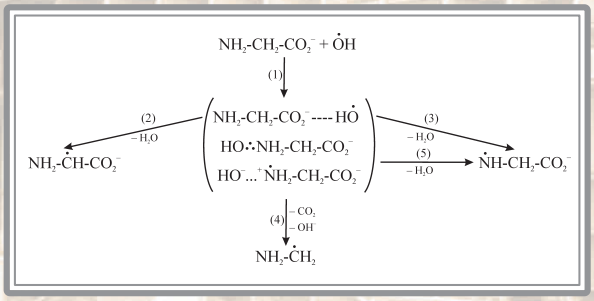


Figure 1. Radical products in the reaction of glycine anions with hydroxyl (OH) radicals.

Novel packing models of AOT Na salt and its alkylammonium complexes

Bis(2-ethylhexyl)-sulfosuccinate sodium salt, AOT, is a widely used anionic surfactant, and its lyotropic properties have been studied extensively. Pure AOT forms a hexagonal columnar phase, involving a highly ordered structure with each column cross-section containing three tessellated molecules in the plane normal to the column axis. The structure is trigonal locally, but hexagonal over the long range. At subambient temperatures the AOT–alkylammonium complexes (C_n-AOT, n=10-16) also display a hexagonal columnar phase, but this is more disordered and each column cross-section contains only two ion pairs (Ungar et al., 2009).

Mechanism of quantum effects in hydrogen-bonded ferroelectric crystals

In this work we considered the mechanism of quantum paraelectricity and the complete H/D isotope effect in hydrogen-bonded crystals of the $K_3H(SO_4)_2$ group. These quantum effects are commonly attributed to proton tunneling and the geometric isotope effect, but their complete mechanism cannot be ascertained because the neutron scattering experiments indicate contradictory hydrogen-bond proton potentials. We suggested a simple model that can explain both the quantum effects and contradictory experimental results (Merunka et al., 2009).

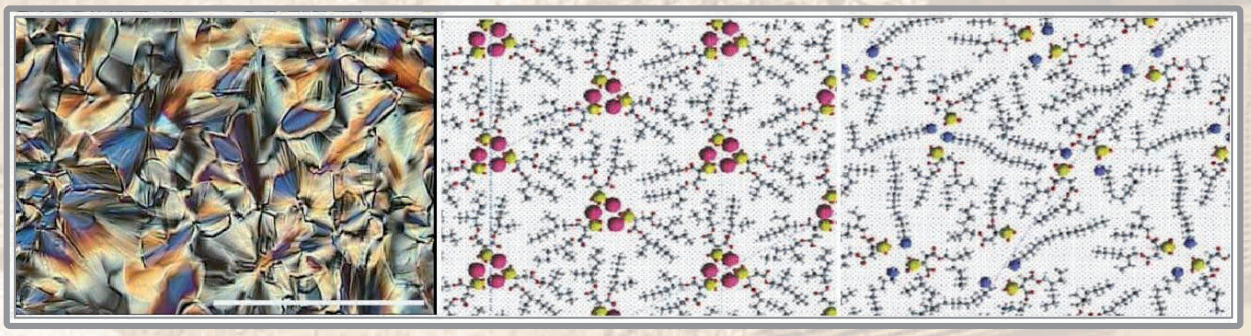


Figure 2. Left: Optical micrograph of AOT-decylammonium salt. The texture is formed upon cooling from isotropic liquid. Scale bar = 100 μm. Middle: Snapshots of molecular dynamics (MD) simulations of AOT Na salt. Right: Snapshots of MD simulations of C_{14}-AOT.

π-Stacking of quinoid rings in crystals of alkali diaqua hydrogen chloranilates

A potent oxido/reduction property makes quinones widely used by nature for bioenergetic processes in living organisms. Among them 2,5-dichloro-3,6-dihydroxy-benzoquinone (chloranilic acid) and its salts or derivatives were selected to study their noncovalent interactions, in particular, hydrogen bonds and π–π interactions. Stacking interactions of quinoid rings, described for the first time, are strikingly different to those of aromatic systems. They can be stacked in an ideal face-to-face fashion with separation distances being significantly smaller than the sum of van der Waals radii (Molčanov et al., 2009).

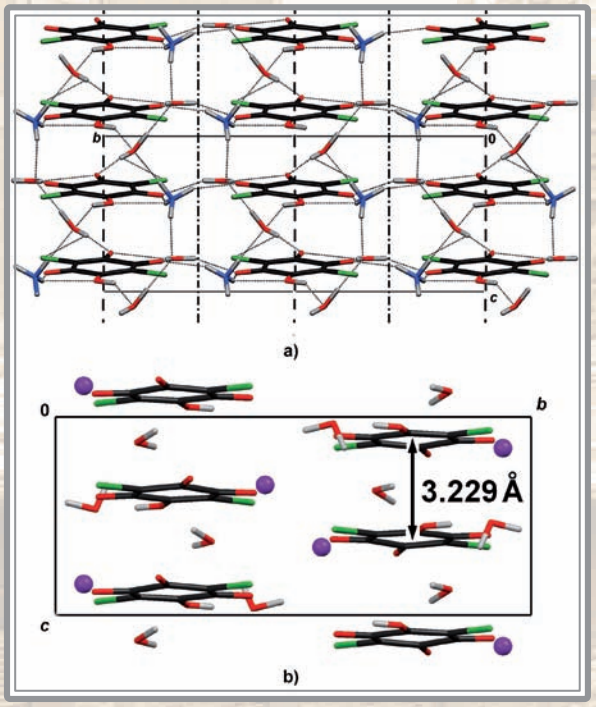


Figure 3. π···π Stacking of quinoid rings observed in crystals of (a) ammonium hydrogen chloranilate dihydrate and (b) potassium hydrogen chloranilate dihydrate.

Methane confined inside water nanocages

We developed a computational methodology for the calculation of coupled translational-rotational states of a molecule confined into or bounded to a much heavier entity (Matanović et al., 2009). The program was used to study the dynamical properties of methane inside nanocages of water hydrates and hydrogen bonded in nanopores of different metal-organic frameworks. These calculations play a significant role in determining the hydrogen binding energies and may provide a possible path towards future hydrogen storage technology.

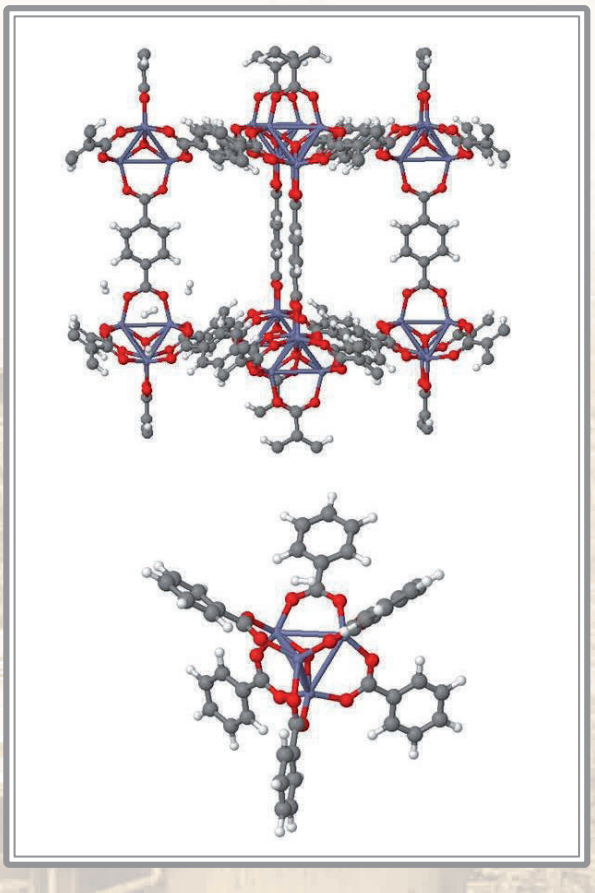


Figure 4. Top: The metal-organic framework-5 (MOF-5) of composition $Zn_4O(BDC)_3$ (BDC=1,4-benzenedicarboxylate). Bottom: part of a framework with a hydrogen bonded to an alpha site.

Crystal structure of the single-stranded DNA-binding protein

Single-stranded DNA-binding (SSB) proteins are involved in the replication, recombination and repair of DNA. Due to their importance in maintaining genomic integrity, they are indispensable for all cellular life. We reported the first crystal structure of the SSB

from a member of the genus Streptomyces at 2.1 Å (Štefanić et al., 2009). It was predicted to be the most stable of the structurally characterized bacterial or human mitochondrial SSBs.

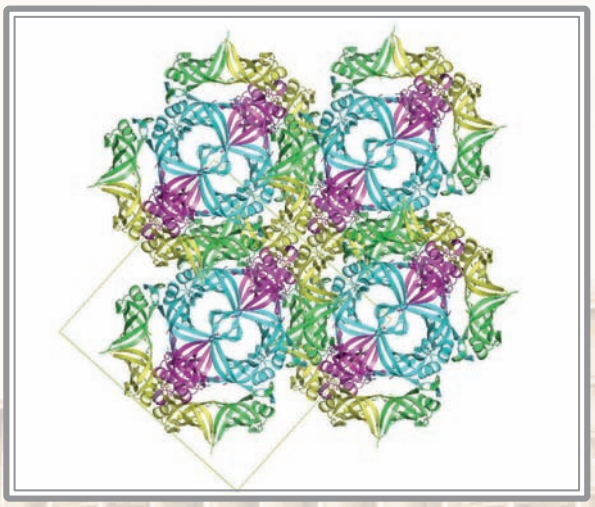


Figure 5. Packing of tetramers in the crystal of the single-stranded DNA-binding protein from Streptomyces coelicolor. Biologically active molecule is composed of four identical chains (in different colors). The view is down the crystallographic c axis in the space group I 222.

AWARDS AND RECOGNITION

The Emily M. Gray Award was given to Professor Greta Pifat-Mrzljak by the American Biophysical Society for significant contributions to education in biophysics in the context of her organization of International Summer Schools on Biophysics since 1981.

Ivan Ljubić: Marie Curie Research Training Network Postdoctoral Fellowship Award, University of Oxford, UK (2009-2010).

Ivana Matanović: UKF Grant in Gaining Experience Programme, Postdoctoral Fellowship for project "Full-Dimensional Quantum Translation-Rotation Dynamics of Methane in Clathrate Hydrates".

EDUCATION

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

PROJECTS

Projects supported by the Ministry of Science, Education and Sport

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

Research, developmental and international projects

1. Chemical applications of advanced ESR-techniques, B. Rakvin (Bilateral project with Austria)
2. Application of MALDI mass spectrometry in protein and intact cell analysis: characterisation of the novel SGNH-hydrolase family from Streptomyces and mapping of Fusanium parasites, I. Leščić Ašler (Bilateral project with Austria)

3. Theoretical study of the reactivity of metallo centres in proteins, S. Tomić (Bilateral project with Austria)
4. Enzyme catalysis-model systems: Proton transfer in low barrier hydrogen bonds, B. Kojić-Prodić (Bilateral project with Slovenia)
5. Development of new algorithms for the analysis of protein active sites, Z. Štefanić (Bilateral project with Slovenia)
6. Theoretical study of enzyme reactions, S. Tomić (Bilateral project with Slovenia)
7. Ozone Pollution Index and National Air Quality Standard, L. Klasinc (Bilateral project with China)
8. "Investigations of calcium phosphate based biomaterials", Maja Dutour Sikirić (FP6 Specific Support Action "Creating international cooperation teams of excellence in the field of emerging biomaterial surface research")
9. Advanced Paramagnetic Resonance Methods in Molecular Biophysics, Boris Rakvin (COST physics P-15 action)

SELECTED INVITED LECTURES

1. Valić S. ESR - Spin probe method in studying nanocomposite rubber materials. International Conference of Hi-Tech Materials: ICHTM-09, Kharagpur, India, February 11-13, 2009.
2. Klasinc L, Cvitaš T, De Marco A, Kezele N, Paoletti E. Rating of Mediterranean air pollution monitoring sites. 15th International Symposium on Environmental Pollution and its Impact on Life in the Mediterranean Region, Bari, Italy, October 7-11, 2009.
3. Ljubić I. Towards understanding mechanism of reversible hydrogen storage in transition metal doped sodium alanate. Hydrogen for the Future, Warsaw, Poland, October 21-25, 2009.
4. Bosanac S. Atoms in an electromagnetic field. ETH, Zurich, Switzerland, December 04, 2009.
5. Ilakovac Kveder M. From LDL to soft condensed matter. 4th Christmas Biophysics Workshop (XBW 2009), Seggau Castle, Leibnitz, Austria, December 14-15, 2009.

SELECTED ORGANIZED CONFERENCES

1. 3rd Adriatic Meeting on Computational Solutions in the Life Sciences, Primošten, September 1-5, 2009, organized jointly by S Tomić, D Babić, and N Došlić (ZFK) and D Smith (ZOKB).
2. 10th International Summer School on Biophysics "Supramolecular Structure and Function", Rovinj, September 19 – October 1, 2009.

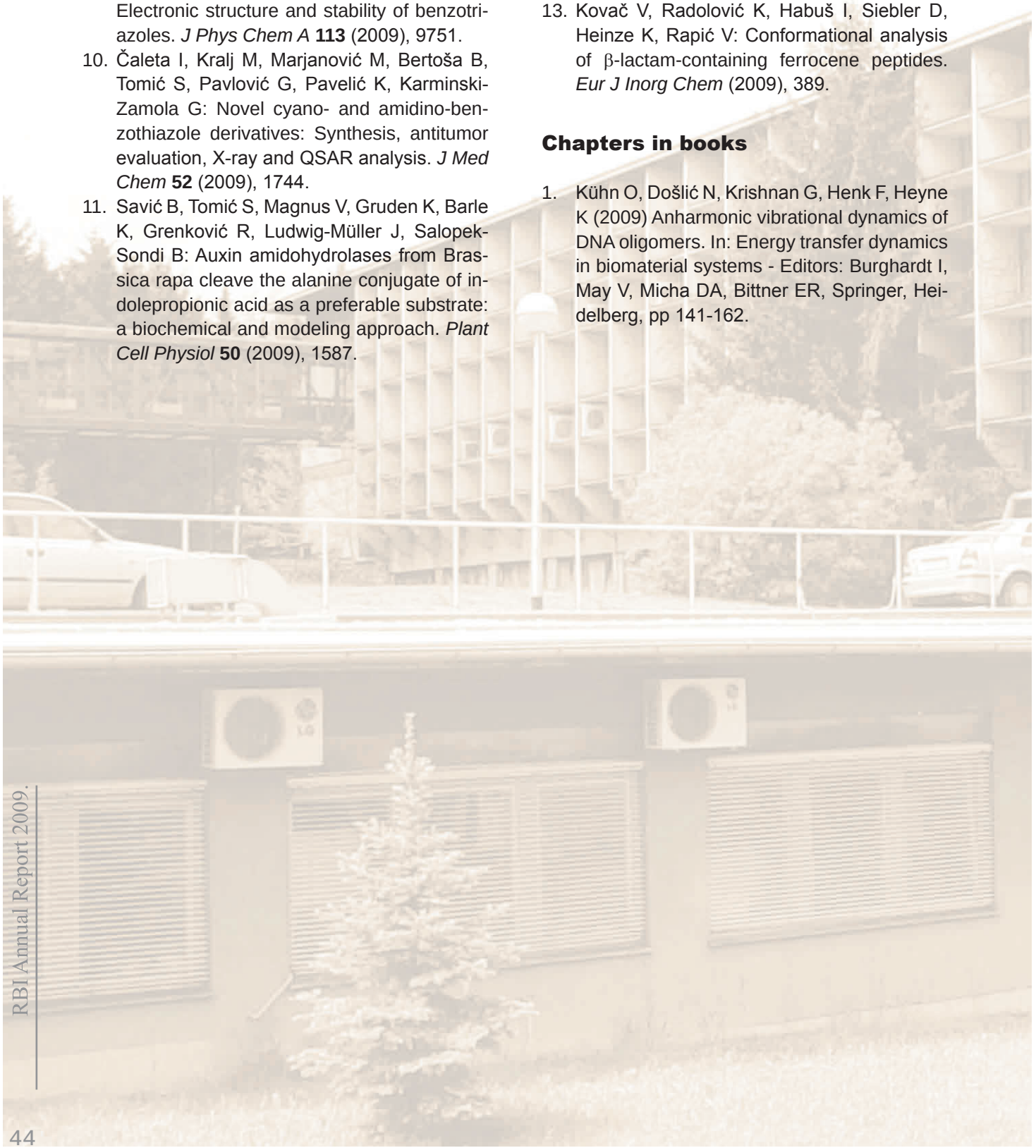
SELECTED PUBLICATIONS

1. Štefanić I, Ljubić I, Bonifačić M, Sabljić A, Asmus K-D, Armstrong DA: A surprisingly complex aqueous chemistry of the simplest amino acid. A pulse radiolysis and theoretical study on H/D kinetic isotope effects in the reaction of glycine anions with hydroxyl radicals. *Phys Chem Chem Phys* **11** (2009), 2256.
2. Ungar G, Tomašić V, Xie F, Zeng X-B: Structure of liquid crystalline aerosol-OT and its alkylammonium salts. *Langmuir* **25** (2009), 11067.
3. Molčanov K, Kojić-Prodić B, Meden A: π-Stacking of quinoid rings in crystals of alkali diaqua hydrogen chloranilates. *Cryst Eng Comm* **11** (2009), 1407.
4. Merunka D, Rakvin B: Mechanism of quantum effects in hydrogen-bonded crystals of the $K_3H(SO_4)_2$ group. *Phys Rev B* **79** (2009), 132108.
5. Kveder M, Merunka D, Jokić M, Makarević J, Rakvin B: Electron spin-lattice relaxation in solid ethanol: The effect of nitroxyl radical hydrogen bonding and matrix disorder. *Phys Rev B* **80** (2009), 052201.
6. Matanović I, Xu M, Moskowitz J, Eckert J, Bačić Z: Methane molecule confined in the small and large cages of structure I clathrate hydrate: Quantum six-dimensional calculations of the coupled translation-rotation eigenstates. *J Chem Phys* **131** (2009), 224308.
7. Štefanić Z, Vujaklija D, Luić M: Structure of the single-stranded DNA-binding protein from Streptomyces coelicolor. *Acta Crystallogr D* **65** (2009), 974.

8. Mališ M, Matanović I, Došlić N: A computational study of electronic and spectroscopic properties of formic acid dimer isotopologues. *J Phys Chem A* **113** (2009), 6034.
9. Novak I, Abu-Izneid T, Kovač B, Klasinc L: Electronic structure and stability of benzotriazoles. *J Phys Chem A* **113** (2009), 9751.
10. Čaleta I, Kralj M, Marjanović M, Bertoša B, Tomić S, Pavlović G, Pavelić K, Karminski-Zamola G: Novel cyano- and amidino-benzothiazole derivatives: Synthesis, antitumor evaluation, X-ray and QSAR analysis. *J Med Chem* **52** (2009), 1744.
11. Savić B, Tomić S, Magnus V, Gruden K, Barle K, Grenković R, Ludwig-Müller J, Salopek-Sondi B: Auxin amidohydrolases from Brassica rapa cleave the alanine conjugate of indolepropionic acid as a preferable substrate: a biochemical and modeling approach. *Plant Cell Physiol* **50** (2009), 1587.
12. Dutour Sikirić M, Gergely C, Elkaim R, Wachtel E, Cuisinier FJG, Füredi-Milhofer H: Biomimetic organic-inorganic nanocomposite coatings for titanium implants. *J Biomed Mater Res A* **89** (2009), 759.
13. Kovač V, Radolović K, Habuš I, Siebler D, Heinze K, Rapić V: Conformational analysis of β-lactam-containing ferrocene peptides. *Eur J Inorg Chem* (2009), 389.

Chapters in books

1. Kühn O, Došlić N, Krishnan G, Henk F, Heyne K (2009) Anharmonic vibrational dynamics of DNA oligomers. In: Energy transfer dynamics in biomaterial systems - Editors: Burghardt I, May V, Micha DA, Bittner ER, Springer, Heidelberg, pp 141-162.



Division of Organic Chemistry and Biochemistry

ZOKB

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

DIVISIONAL ORGANIZATION

Head: Kata Majerski

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

- Laboratory for stereoselective catalysis and biocatalysis, Zdenko Hameršak
- Laboratory for synthetic organic chemistry, Kata Majerski
- Laboratory for supramolecular and nucleoside chemistry, Mladen Žinić
- Laboratory for carbohydrate, peptide and glycopeptide chemistry, Lidija Varga-Defterdarović
- Laboratory for cellular biochemistry, Marija Abramić
- Laboratory for physical organic chemistry, Mirjana Eckert-Maksić
- Laboratory for molecular spectroscopy, Goran Baranović
- Laboratory for study of interactions of biomacromolecules, Ivo Piantanida
- Group for quantum organic chemistry, David Smith

OVERVIEW OF THE DIVISION

In 2009, the members of the Division continued to maintain their established excellence in scientific research. As in previous years, the principal focus was directed towards basic research in the fields of organic and bioorganic chemistry. Over 52 contributions 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, and quantum organic chemistry. In addition to the fundamental research, 2 patent applications were submitted. 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 6 B.Sc. and 3 Ph.D theses. The Division's scientists were also active in national and international societies and bodies and served as editors or members of several editorial boards.

TOP ACHIEVEMENTS

New Concept in Superbase Design – A Flexible Bis–Guanidino Compound

In a joint computational–experimental study it was shown that a combination of two

hpp fragments (hppH = 1,3,4,6,7,8-hexahydro-2H-pyrimido[1,2-a]pyrimidine, Figure 1) connected together by a flexible methylene group yields a very strong superbase. Its proton affinity of 270.6 kcal mol^{-1} in the gas–phase and the corresponding pKa value of 28.98 ± 0.05 in acetonitrile are astoundingly high. Difference electron density maps generated from high-resolution X-ray diffraction studies at 110 K gave the first direct experimental evidence for proton transfer in a poly(guanidino) system, Figure 1. (Coles et al., 2009).

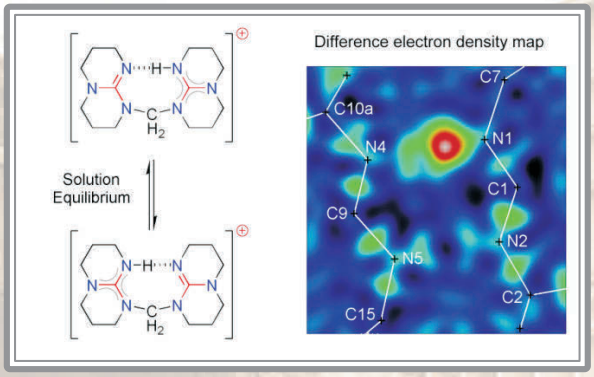


Figure 1. A new flexible bicyclic superbase with its X-ray diffraction analysis offering the first direct experimental evidence for proton transfer in a poly(guanidino) system.

Photoinduced domino reactions

Adamantyl-phthalimides undergo photochemical reactions upon direct irradiation and triplet sensitization and, in this way, give rise to new products (Figure 2). Besides formation of the primary photoproducts, the first photochemical step initiates a domino sequence of a thermal and a photochemical reaction. The latter involves two photochemical intramolecular γ-H abstractions, which are delivered stereospecifically to the hexacyclic benzazepine products. The formation of products can be explained by intramolecular H-abstraction from the (alkyl) adamantane to the excited phthalimide, either from the excited singlet state or from a hidden upper excited triplet state (Horvat et al., 2009).

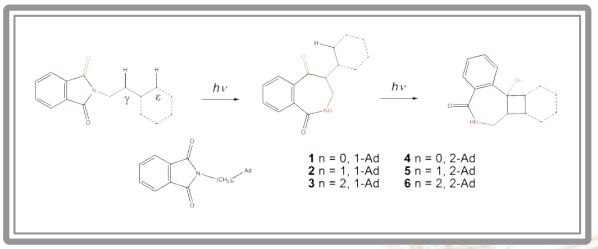


Figure 2. Photoinduced domino reactions of Adamantyl-phthalimides.

Photodissociation of the peptide bond

In a continuation of computational studies of ultrafast phenomena in photobiology, dynamics simulations of the dissociation of the peptide bond in *N,N*-dimethylformamide, following excitation to the lowest excited states, was explored. It was shown that methyl groups have a profound effect on the lifetime, as well as on the percentage of trajectories that remain undissociated in the S_1 state during simulations (Eckert-Maksić et al., 2009).

Solid-state complexation of anions by adamantyl calyx[4]pyrroles

Novel adamantane derivatives of calix[4]pyrrole and calixphyrin have been synthesized. The structures have been characterized by X-ray powder diffraction, and single crystal X-ray analysis (Figure 3). It was found that an adamantane derivative of calix[4]pyrrole forms complex with Cl^-, both in the solid state and in DMSO solution. The solid state complexation, which is the first example of such complex formation with an anion in the

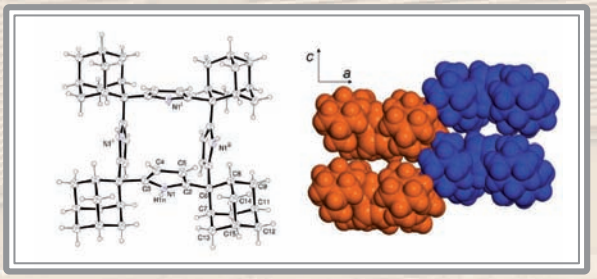


Figure 3. ORTEP view of adamantyl calyx[4]pyrrole (left). Crystal packing of adamantyl calyx[4]pyrrole (right).

solid state, was accomplished by grinding in a mill (Aleškoviće et al., 2009).

Controlled self-assembly of chiral gelator molecules into aligned fibers induced by nematic to smectic B phase transitions

Chiral bisoxalamide (Figure 4, **1**) shows a remarkable gelling capacity of nematic and smectic B liquid-crystalline phases of heptylcyclohexanecarboxylic acid (HCC, Figure 4, **2**). The chiral nematic gel, which contains left-handed helical fibre bundles, is formed if the gelator is present in amounts higher than 0.5 wt% (Figure 4, TEM image **A**). At lower amounts of **1**, no nematic gel forms. However, the nematic to smectic B phase transition triggers instantaneous self-assembly of the gelator molecules into aligned fibers (Figure 4, TEM image **B**). The latter liquid crystalline gel system represents an example of controlled self-assembly induced by an LC phase transition. The results may open new possibilities for preparation of LC phase-controlled self-assembled systems and the production of unidirectionally aligned assemblies (Šijaković-Vujičić et al., 2009).

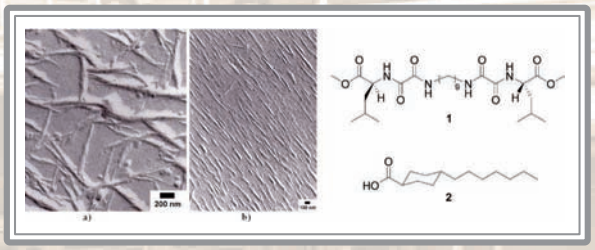


Figure 4. TEM images (Pd shadowing) of 1/2 LC gels: a) chiral nematic gel showing left handed helical bundles, and b) highly oriented fiber assemblies formed in the smectic B gel at 0.5 wt% of gelator 1.

Stereoisomeric bis(phenylglycinol) malonamide gelators: rare examples of gelling *meso*-compounds

Bis(phenylglycinol)malonamide (Figure 5, **1**), and methyl-, dimethyl-, ethyl-, diethyl- and isopropylmalonamides (Figure 5, **2**, **3**, **4**, **5** and **6**) exhibited profoundly different gelling properties. While monoalkyl malonamides are efficient organogelators, the symmetrically substituted dialkymalonamides (*R,R*)-dimethylmalonamide **3** and (*R, R*)-diethylmalonamide **5**, as well as the unsubstituted **1**, are devoid of any gelation ability. In contrast to all earlier published observations that *meso*-diasteroisomers lack any gelation ability, the m*eso*-diastereoisomers (*R, r, S*)-**2** and (*R, s, S*)-**2**, as well as (*R, r, S*)-**4** and (*R, s, S*)-**4**, each possessing a pseudoasymmetric centre, represent very rare examples of gelling *meso*-compounds (Jokić et al., 2009).

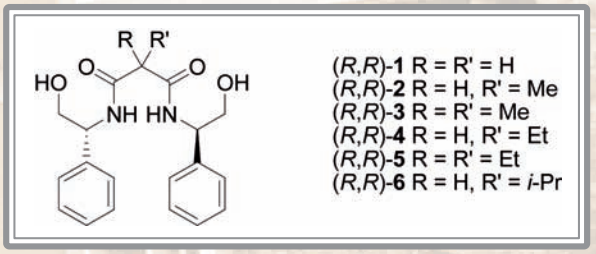


Figure 5. Structures of bis(phenylglycinol)malonamide gelators.

Inversion of enantioselectivity in quinine-mediated desymmetrization of glutaric meso-anhydrides

An unexpected inversion of enantioselectivity, dependent on the level of quinine loading, was observed during the desymmetriza-

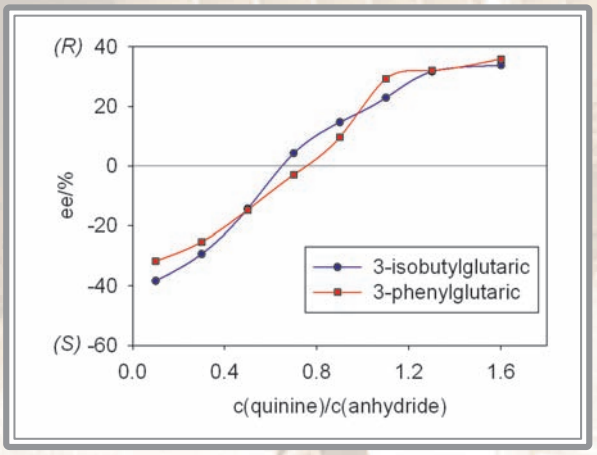


Figure 6. Influence of quinine loading on the desymmetrization of 3-substituted glutaric anhydrides.

tion of glutaric *meso*-anhydrides. Decreasing the catalyst loading from 1.6 equivalents to 0.1 equivalent caused a clear inversion of stereochemistry - from about 40% ee of *R*-configuration to about 40% ee of the opposite one (Figure 6).The study of carboxylic acid additives revealed that enantioselectivity can be increased to >60% ee of *S*-product. This represents a level of enantioselectivity that might be of synthetic interest (Ivšić et al., 2009).

The Sonogashira Cross-Coupling Reaction

It was demonstrated that aliphatic amino-acid-derived acetylenes and chlorides can be successfully applied in the Sonogashira type of cross-coupling reactions. Although the reactions must be performed under rigorous conditions and yields are lower than those obtained with aromatic substituents, the presented results encourage further utilization of the Sonogashira reaction (Gredičak et al., 2009).

Synthesis of novel porphyrin-shaped cavities

In the context of studies of 1,3-dipolar cycloaddition reactions, several novel hinged porphyrin-spacer-acceptor dyads and doubly-hinged POR-spacer-POR cavity shaped scaffolds were prepared. The strategy involved the coupling of norbornene building BLOCKs, formed by the Diels-Alder reaction of porphyrin 1,3-dienes with norbornadiene derivatives, with an ester-activated cyclobutene epoxide BLOCK (Figure 7), (Tang et al., 2009).

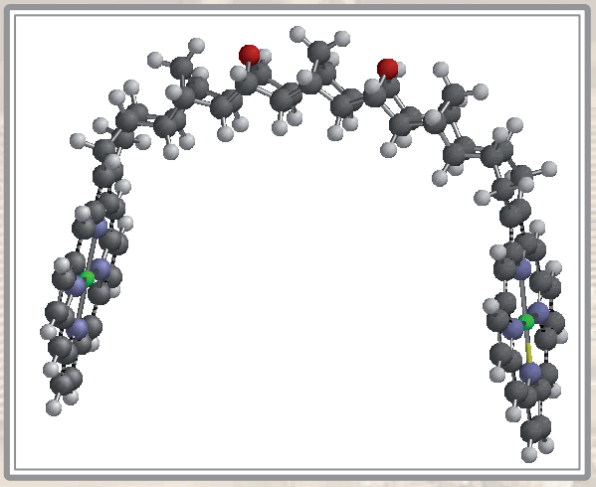


Figure 7. AM1-optimized structure of novel bis-porphyrine scaffold

Target chemical transformations of peptides

Chemical transformed peptides were produced by the replacement of the Gly_2 residue in leucine and methionine enkephalins (Tyr-Gly-Gly-Phe-Leu/Met) with side-chain glucosylated or adamantylated D/L-aspartic or -glutamic acids. It was shown that the synthesized compounds modestly inhibited the growth of the tumour cells and one of them,Tyr-D-Glu(AdNH)-Gly-Phe-Met, showed significant antiproliferative activity, somewhat more pronounced on MCF-7 (breast carcinoma) and MOLT (lymphoblastic leukemia) cells (Horvat et al., 2009).

Phase transition temperatures in a minute

A rapid, inexpensive method for obtaining phase transition temperatures, completely free of any personal bias, was proposed. The method is based on absolute variations

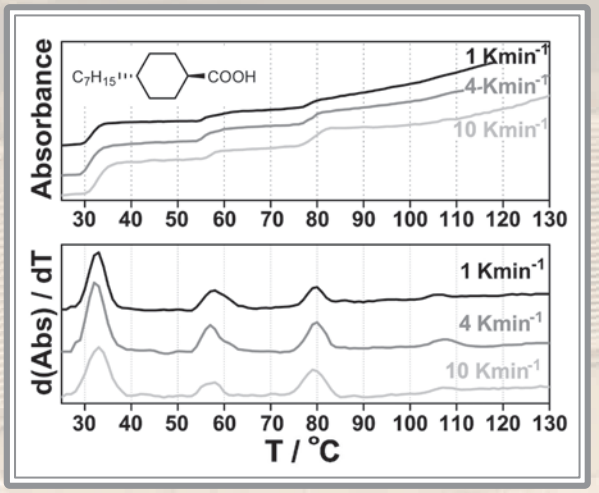


Figure 8. Above room temperature trans-4-heptylcyclohexanecarboxylic acid can be in five solid phases (measurement with less than 2 mg of the sample in approximately 15 min).

of the baseline in temperature-dependent mid-infrared transmittance spectral data (Figure 8). The approach offers great prospect as an economical way of establishing critical temperature regions for analytical and quality control purposes (Zimmermann and Baranović, 2009).

Mechanism-Based Inactivation of Glycerol Dehydratase

Glycerol dehydratase (GDH) is an important coenzyme-B_{12}-depedent enzyme that catalyzes a key step in the biotechnological conversion of glycerol to 1,3-propanediol, which is used to produce textile fibres. Computational studies of the reaction of GDH with but-3-ene-1,2-diol characterized a number of radical intermediates that could be responsible for the inactivation observed with this substrate analogue and thus contributed to the advancement of mechanistic understanding of this industrially relevant process (Sandala et al., 2009).

Novel monomethine cyanine dyes for DNA/RNA

Comparison of the binding properties of a series of monomethine cyanine derivatives (Figure 9) to ds-DNA and ds-RNA revealed a significant impact of the properties of the substituent attached to the longer axis of the aromatic core. Namely, only compounds characterised by a length of the longer axis not exceeding the length of the longer axis of basepairs could intercalate into ds-DNA and ds-RNA. The consequent ds-RNA over ds-DNA selectivity is a most appealing and rather rare property among small molecules. The interactions with ss-RNA were strongly dependent on both the structure of compound and the base composition of RNA. The studied compounds revealed considerable antiproliferative activity against solid tumours and especially toward haematological malignancies (IC50 = 0.001–6.6 lM), whereby normal human aortic endothelial cells (HAEC) were significantly less affected. Results of uptake and intracellular distribution of compounds in living cells showed that the binding is not primarily to nuclear DNA but their fluorescence is scattered throughout the entire cells (Glavaš-Obrovac et al., 2009).

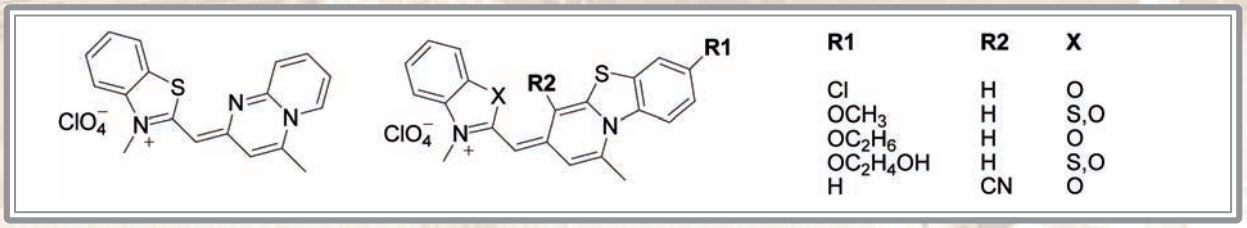
Study of structure-function relationship in metallopeptidase family

The role of the unique, fully conserved tryptophan residue in proteins of the M49 metallopeptidase family was investigated by site-directed mutagenesis. The obtained results indicate the importance of this amino acid in maintaining the functional integrity of enzymes' S2 subsite (Špoljarić et al., 2009).

PATENTS

DZIV P20090186A. Basarić N, Blažek V, Majerski K. Adamantane bisurea derivatives, method of preparation and applications in anion sensing.

EP 1786763. Maksić M, Glasovac Z. N,N',N''-Tris-(3-dimethylaminopropyl)-guanidine, the procedure of preparation from carbodiimide and application in reactions of transesterification of oil.



R1	R2	X
Cl	H	O
OCH_3	H	S,O
OC_2H_6	H	O
OC_2H_4OH	H	S,O
H	CN	O

Figure 9. Studied monomethine cyanine derivatives.

NEW EQUIPMENT

High Temperature ATR Accessory for a FT IR spectrometer

EDUCATION

The Division provides annually over 25 undergraduate and graduate courses at universities Zagreb, Rijeka, Osijek and Dubrovnik.

AWARDS AND RECOGNITION

Zvonimir Maksić: National Science Award of the Republic of Croatia for the Lifetime Achievements in the field of Natural Sciences

Nikola Basarić: Leopold Ružička Award for young scientists of the Croatian Chemical Society.

Ina Nemet: Juvenile Diabetes Research Foundation Postdoctoral Fellowship Award,

Novel Pathways of Glycation Damage in Diabetic Complications (2008-2010).

Matija Grdičak, Doctoral Students Fellowship from the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia: New Methods for the Synthesis of Photoactive Enediynes (January-April, 2009).

Ivana Antol, Postdoctoral Fellowship from the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia: Theoretical Study of the Biologically Relevant Photochemical Reaction (01.03.2009 - 01.03.2010).

The best poster awards

Antol I. et al. "Excited state potential energy curves by single reference TD-B2PLYP and SCS-CIS (D) methods". 5th Symposium on Theoretical Chemistry, Neuss am Rhein, Germany, 8-12 September 2009.

Štrukil V. et al., "A Mechanochemical Approach Towards Solvent-Free Synthesis" Symposium on Mechanochemistry and Solvent-Free Synthesis, Queen's University Belfast, UK, 6-7 November 2009.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. Molecular enzymology and protein interactions of hydrolases, Marija Abramić
2. Macrocyclic ligands, structures in solutions and molecular spectroscopies, Goran Baranović
3. Organic and bioorganic processes in ground and excited states, Mirjana Eckert-Maksić
4. Chiral building blocks for biologically active molecules. Synthesis and reactivity, Zdenko Hameršak
5. Chemical transformations of natural compounds, Lidija Varga-Defterdarović
6. Cage compounds: Building blocks for molecular architecture, Kata Majerski
7. Brønsted and Lewis acids and bases in chemistry and biochemistry, Zvonimir Maksić
8. Host-guest interactions in policyclic systems, Davor Margetić
9. Design, synthesis and study of interactions of small molecules with DNA, RNA and proteins, Ivo Piantanida
10. Computational studies of protein structure and function, David Smith
11. Chiral organic materials - synthetic, structural and functional research, Vladimir Vinković
12. Synthesis of novel biologically active nucleobase and nucleotide derivatives, Biserka Žinić
13. Supramolecular chemistry of gels. Self-assembly approach to functional hybrid materials, Mladen Žinić

Research, developmental and international projects

1. Synthesis and photochemistry of polycyclic derivatives of phenols: potential precursors for long-lived quinone methides, Nikola Basarić (UKF 3A Grant Agreement 46/09).

2. Fluorescent Anion Sensors: Synthesis and Spectroscopic Characterization, Nikola Basarić (Croatian-China bilateral project).
3. Quinone methides: Potential Anticancer Agents (till June 19th.), Croatian Academy of Science and Arts, Nikola Basarić.
4. Photodynamical simulation of bioorganic processes, Mirjana Eckert-Maksić (Croatian-Austrian bilateral project).
5. Siteselectivity of Protonation of Some organic Molecules of Importance in Chemistry and Biochemistry, Mirjana Eckert-Maksić, (Croatian-Italian bilateral project).
6. Polyfunctional Guanidines. Design, Synthesis and Catalytic Properties of Novel Superbases (till June 19th.), Croatian Academy of Science and Arts, Zoran Glasovac.
7. Artificial Receptors for Bacillus anthracis Specific Anthrose Detection. NATO Science for Peace and Security Programme; CBP.EAP.SFP.983154. (2008-2011) Andreja Jakas and Predrag Čudić.
8. Metal-binding ability of Leu-enkephalin, related glycoconjugates and peptidomimetics: comparative CD and FTIR spectroscopic studies, Andreja Jakas (Croatian-Hungarian bilateral project).
9. Thermally processed foods: possible health implication. COST 927, WG1 and WG5 (2004-2009) Štefica Horvat and Andreja Jakas.
10. Synthesis of carboxyphenyl derivatives (CP-derivatives), Kata Majerski, TECNA s.r.l. Area di Ricerca, Padriciano, Trieste, Italy Projekt no. RI-GM-LG-08-054v01.
11. Biocatalytic application of halohydrin dehalogenases for production of chiral building blocks, Maja Majerić Elenkov (UKF 3A Grant Agreement 51/09).
12. Protein engineering of halohydrin dehalogenases for the production of fine chemicals and pharmaceutical intermediates, Maja Majerić Elenkov (Croatian-Chinese bilateral project).
13. Computer-assisted Design of Strong and Ultra-strong Bases and their Applications, Zvonimir Maksić (Croatian–Germany bilateral project).
14. Design and synthesis of novel aryl-guanidiniocarbonyl-pyrroles, and study of their interactions with DNA/RNA. Ivo Piantanida Croatian–Germany bilateral project)
15. Reinforcement of the Centre for Computational Solutions in the Life Sciences, David Smith (6th Framework Programme, EU–FP6–043749–ReCompSoLS).
16. Computational Prediction of Structure and Catalytic Activity of New Organic Superacids, Robert Vianello (UKF, APO Environmental Protection Services Ltd. Zagreb, Grant Agreement No. 20/08).
17. Acid–Base and Tautomeric Properties of Biologically Relevant Compounds in Solution, Robert Vianello (Croatian–Slovenian bilateral project).
18. The Amide Linkage and its Implications in Molecular Biology, Robert Vianello (Croatian–Austrian bilateral project).
19. COST D31: Organising Non-Covalent Chemical Systems with Selected Functions, Mladen Žinić

SELECTED INVITED LECTURES

1. Piantanida I, Recognition of various DNA / RNA sequences by 4, 9-diazapyrenium and bis-phenanthridinium derivatives in aqueous media. "The 2nd International Workshop-Cum-Training Course on Molecular Medicine and Drug Research", Karachi, Pakistan, January 12 – 15, 2009.
2. Piantanida I. Methods in Studies of Interactions of Small Organic Molecules with Various DNA and RNA Polynucleotides. "Workshop for students of International Center for Chemical and Biochemical Sciences", University of Karachi, Pakistan, January 16, 2009.
3. Piantanida I. Structural tuning of small molecules for non-covalent recognition of specific DNA and RNA sequences, RWTH Aachen University, Institut für Organische Chemie, Aachen, Germany, March 27th, 2009.
4. Smith DM. A Computational Investigation of Glycerol Dehydration: to B_{12} or Not to B_{12}. "21st Croatian Meeting of Chemists and Chemical Engineers", Trogir, Croatia, April 19–22, 2009.
5. Vianello R. Computational Prediction of New

Extremely Acidic Superacids Awaiting Experimental Synthesis. "21st Croatian Meeting of Chemists and Chemical Engineers", Trogir, Croatia, April 19–22, 2009.

6. Vianello R, With computers towards new superacids. "Science Festival 2009", Rijeka, Croatia, April 20–25, 2009.
7. Smith DM, A Computational Perspective on Glycerol Dehydration: To B_{12} or not to B_{12}. "The 2009 Gordon Research Conference on Vitamin B_{12} & Corphins", Oxford, England, August 2–7, 2009.
8. Basarić N. Photoinitiated Domino Reactions of Adamantyl-phthalimides, Department of Chemistry, University of Victoria, Canada BC., September 10, 2009.
9. Smith DM, Studying Enzymatic Mechanism with QM/MM Techniques: An Application to the Dehydration of Glycerol. "Seventh International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2009)", Rhodes, Greece, September 29–October 4, 2009
10. Basarić N. Photoinduced domino reactions of adamantyl phthalimides: from the investigation of reaction mechanisms to the applications in synthesis of biologically active molecules, AMACIZ, Faculty of Chemical Engineering and Technology, University of Zagreb, December 7, 2009.

SELECTED ORGANIZED CONFERENCES

1. The 3rd Adriatic Meeting on Computational Solutions in the Life Sciences, Primošten, Croatia, September 1–5, 2009, organized jointly by D Smith (ZOKB) and S Tomić, D Babić, and N Došlić (ZFK).

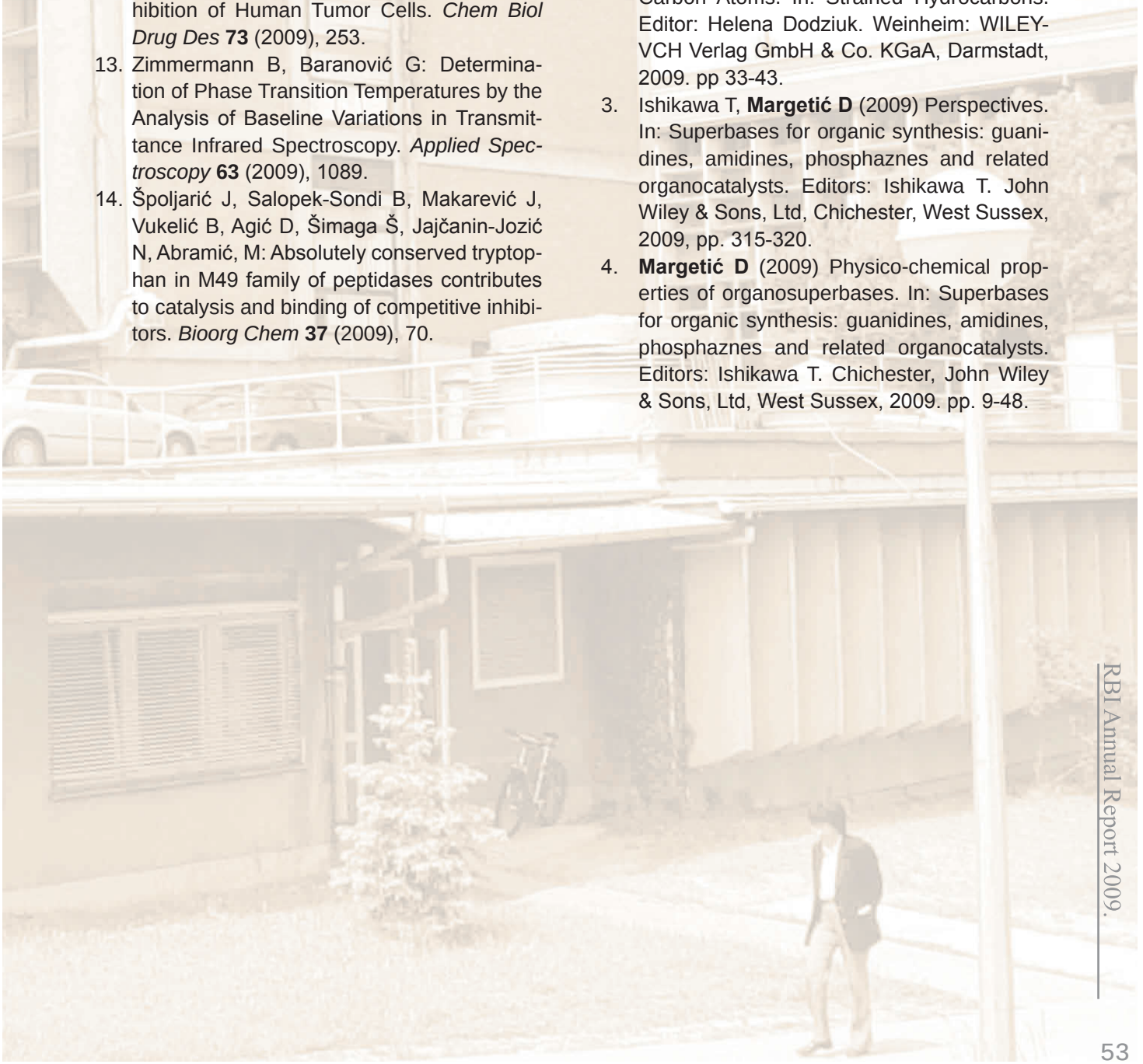
SELECTED PUBLICATIONS

1. Coles MP, Aragón–Sáez PJ, Oakley SH, Hitchcock PB, Davidson MG, Maksić ZB, Vianello R, Leito I, Kaljurand I, Apperley DC: Superbasicity of a Bis–guanidino Compound with a Flexible Linker: A Theoretical and Experimental Study. *J Am Chem Soc* **131** (2009), 16858.
2. Sandala GM, Kovačević B, Barić D, Smith DM, Radom L: On the Reaction of Glycerol Dehydratase with But–3–ene–1,2–diol. *Chem Eur J* **15** (2009), 4865.
3. Horvat M, Görner H, Warzecha K-D, Neudörfl J, Griesbeck AG, Mlinarić-Majerski K, Basarić N: Photoinitiated Domino Reactions: N-(Adamantyl)phthalimides and N-(Adamantylalkyl)phthalimides. *J Org Chem* **74** (2009), 8219.
4. Glavaš-Obrovac Lj, Piantanida I, Marczi S, Mašić L, Timcheva I, Deligeorgiev TG: Minor structural differences of monomethine cyanine derivatives yield strong variation in their interactions with DNA, RNA as well as on their in vitro antiproliferative activity. *Bioorg Med Chem* **17** (2009), 4747.
5. Alešković M, Halasz I, Basarić N, Mlinarić-Majerski K: Synthesis, structural characterization, and anion binding ability of sterically congested adamantane-calix[4]pyrroles and adamantane-calixphyrins. *Tetrahedron* **65** (2009), 2051.
6. Eckert-Maksić M, Antol I: Study of the mechanism of the N−CO photodissociation in N, N-dimethylformamide by direct trajectory surface hopping simulations. *J Phys Chem A* **113** (2009), 12582.
7. Ivšić T, Z. Hameršak Z: Inversion of enantioselectivity in quinine-mediated desymmetrization of glutaric *meso*-anhydrides. *Tetrahedron: Asymmetry* **20** (2009), 1095.
8. Grdičak M, Jerić I: The Sonogashira Cross-Coupling Reaction of Alkenyl Chlorides with Aliphatic Acetylenes. *Synlett* (2009), 1063.
9. Šijaković-Vujičić N, Šepelj M, Lesac A, Žinić M: Controlled self-assembly of chiral gelator molecules into aligned fibers induced by nematic to smectic B phase transitions. *Tetrahedron Lett* **50** (2009), 4430.
10. Jokić M, Čaplar V, Portada T, Makarević J, Šijaković-Vujičić N, Žinić M: Stereoisomeric bis(phenylglycinol)malonamide gelators: rare examples of gelling *meso*-compounds. *Tetrahedron Lett* **50** (2009), 509.

11. Tang H, Merican Z, Dong Z, Margetić D, Marinić Ž, Gunter MJ, Officer D, Butler DN, Warrener RN: Hinged *bis*-Porphyrin Scaffolds I. The Synthesis of a New Porphyrin Diene and its Role in Constructing Hinged Porphyrin Dyads and Cavity Systems. *Tetrahedron Lett* **50** (2009), 667.
12. Horvat Š, Kralj M, Perc M, Jerić I, Varga-Defterdarović L, Jakas A, Roščić M, Šuman L, Gredičak M: Novel Side-Chain Glucosylated and Adamantylated [Asp^2/Glu^2]Enkephalin Analogs: Synthesis and *In Vitro* Growth Inhibition of Human Tumor Cells. *Chem Biol Drug Des* **73** (2009), 253.
13. Zimmermann B, Baranović G: Determination of Phase Transition Temperatures by the Analysis of Baseline Variations in Transmittance Infrared Spectroscopy. *Applied Spectroscopy* **63** (2009), 1089.
14. Špoljarić J, Salopek-Sondi B, Makarević J, Vukelić B, Agić D, Šimaga Š, Jajčanin-Jozić N, Abramić, M: Absolutely conserved tryptophan in M49 family of peptidases contributes to catalysis and binding of competitive inhibitors. *Bioorg Chem* **37** (2009), 70.

CHAPTERS IN BOOKS

1. Majerić Elenkov M, Tang L, Hauer B, **Janssen DB** (2009) One-pot biocatalytic synthesis of methyl (*S*)-4-chloro-3-hydroxybutanoate and methyl (*S*)-4-cyano-3-hydroxybutanoate. In: Practical Methods for Biocatalysis and Biotransformations – Editors: Whitall J, Sutton P, Wiley, Chipenham, 2009, pp 199-203.
2. **Mlinarić-Majerski K** (2009) Distorted Saturated Hydrocarbons: Molecules with Inverted Carbon Atoms. In: Strained Hydrocarbons. Editor: Helena Dodziuk. Weinheim: WILEY-VCH Verlag GmbH & Co. KGaA, Darmstadt, 2009. pp 33-43.
3. Ishikawa T, **Margetić D** (2009) Perspectives. In: Superbases for organic synthesis: guanidines, amidines, phosphaznes and related organocatalysts. Editors: Ishikawa T. John Wiley & Sons, Ltd, Chichester, West Sussex, 2009, pp. 315-320.
4. **Margetić D** (2009) Physico-chemical properties of organosuperbases. In: Superbases for organic synthesis: guanidines, amidines, phosphaznes and related organocatalysts. Editors: Ishikawa T. Chichester, John Wiley & Sons, Ltd, West Sussex, 2009. pp. 9-48.



Division of Materials Chemistry

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

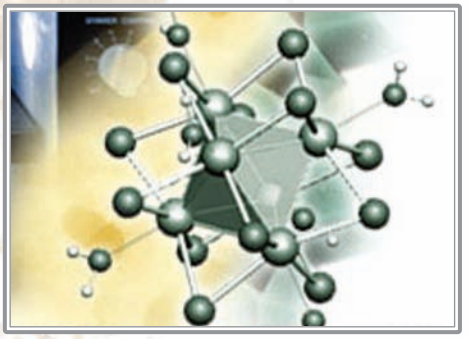
ZKM

DIVISIONAL ORGANISATION

Head: Svetozar Musić

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

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



OVERVIEW OF THE DIVISION

The Division of Materials Chemistry is a centre of excellence in materials science. We investigate the chemical, microstructural and physical properties of various materials. In addition, we develop new methods of materials synthesis. Our primary interests are in metal oxides, glass-ceramics, zeolites, cluster compounds, organic polymers, intermetallic compounds and metal hydrides. There is a long tradition in studies of the kinetics and mechanisms in different precipitation systems. The Radiation Chemistry and Dosimetry Laboratory is the only existing unit in Croatia which covers all aspects of physical-chemical effects of ionizing radiation and their applications. Low-dose and high-dose chemical dosimetry systems were developed and received international recognition. Our main research activities are financially sponsored by the Ministry of Science, Education and Sports. There are also numerous cooperation projects with industry, hospitals, state institutions and faculties.

TOP ACHIEVEMENTS

Synthesis of porous hematite particles

Porous hematite (α-Fe_2O_3) particles were crystallized from dense β-FeOOH suspensions containing different starting concentrations of ammonium amidosulfonate (AAS). The crystallization processes were monitored by XRD, ^{57}Fe Mössbauer and FT-IR spectroscopies and with FE-SEM. FE-SEM demonstrated the importance of the aggregation mechanism in the formation of peanut-type α-Fe_2O_3 particles, as well as in the formation of interconnected (with the neck) double cupolas. The last α-Fe_2O_3 particles were porous and they consisted of linear chains of small α-Fe_2O_3 particles (also interconnected)

which were directed from the center towards the surface of the cupola. Preferential adsorption of sulfonate (later sulfate) groups on selected planes was responsible for the features obtained (Žic et al., 2009).

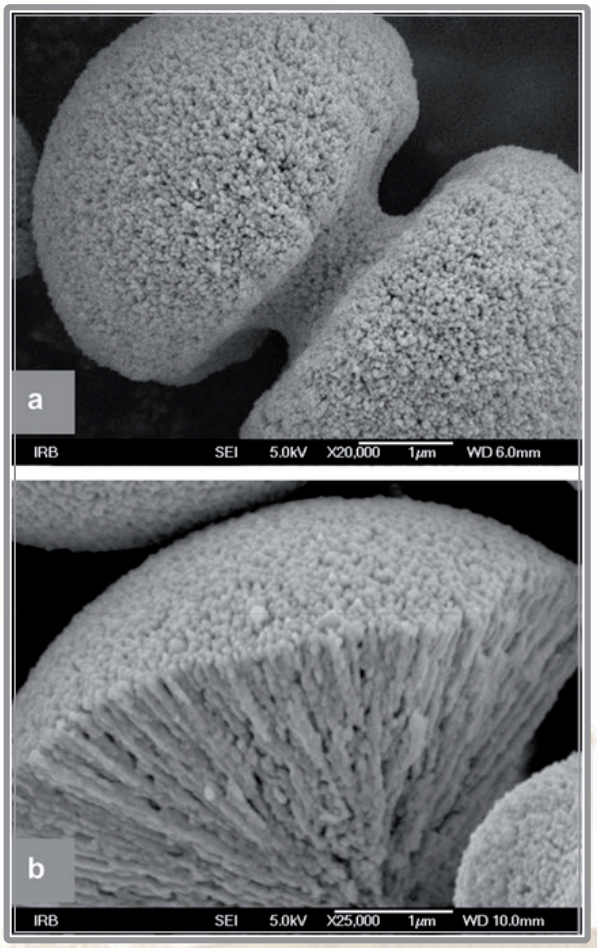


Figure 1. (a) α-Fe_2O_3 double coupla with neck (interconnected) and (b) cross-section of one particle showing the linear chains of interconnected primary α-Fe_2O_3 subparticles.

A Contribution to Understanding the Mechanism of Crystallization of Silicalite-1 in Heterogeneous Systems (Hydrogels)

Analysis of a gel, prepared for crystallization of silicalite-1, by different methods such as powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), light microscopy (LM), scanning-electron microscopy (SEM), transmission electron microscopy (TEM), electron diffraction (ED) and atomic force microscopy (AFM) have shown that the freshly prepared gel represents a " hierarchical structure" in which the largest individual gel aggregates (size 200 nm – 1000 nm, or more) are composed of smaller particles in the size range 40 nm – 80 nm, which represent aggregates of ≤ 10 nm particles. Nuclei formed inside the gel particles and/or small silicalite-1 nanocrystals formed by limited growth of nuclei in the gel matrix, can grow only after their release from the gel dissolved during crystallization, i.e. when they are in full contact with the liquid phase. Growth of silicalite-1 crystals in heterogeneous systems takes place by incorporation of small, partially crystalline 10 nm particles and/or their aggregates (10 nm ≤ D ≤ 40 nm) onto the surface of growing silicalite-1 crystals (see Figure 2).

Figure 2. TEM image of the growing silicalite -1 crystal. Magnification: 160000 x.

Precipitation of calcium carbonate

Despite a considerable amount of research on biomineralization and bioinorganic materials, the exact mechanism of interactions between mineral surfaces and dissolved hydrophilic macromolecules is still not known. Therefore, the specific coordinative interac-

tions between the acidic polypeptides and well-defined calcite crystals were investigated by using poly-L-glutamic and poly-L-aspartic acids as analogues of naturally occurring hydrophilic macromolecules rich in aspartic and glutamic acid residues of certain biominerals. The obtained kinetic data indicated that the role of stereochemical and structural matching between the selected polypeptides and calcite surfaces may be of utmost importance for nucleation of calcite crystals in vitro and for their arrangement into the desired shape, size, and orientation (Njegić Džakula et al., 2009).

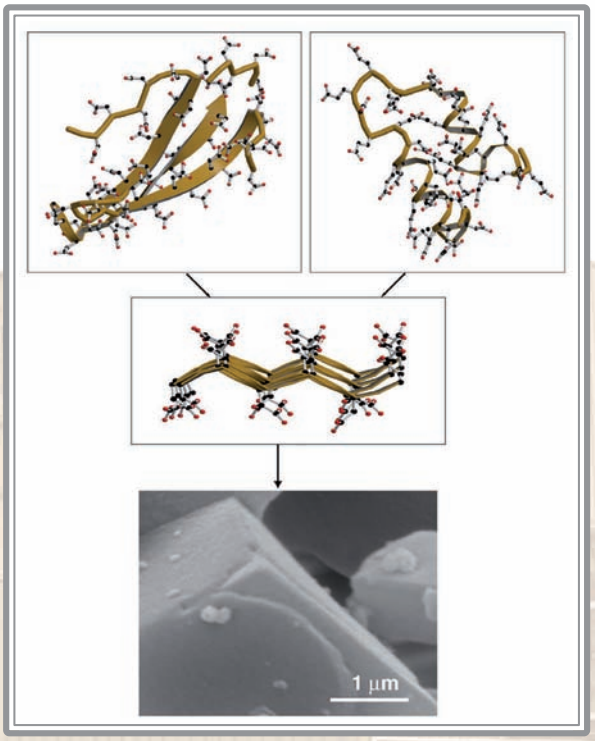


Figure 3. Model of coordinative interaction between side chain carboxylate groups of poly-L-aspartic and poly-L-glutamic acid, assuming extended β-sheet regions, and calcium ions at the calcite surface. Because of stable face growth inhibition, new thermodynamically unstable {hkl} faces appear.

The electronic structure of $RECo_5$ (RE=Nd, Ho, Er and Tm) Intermetallics

The electronic structure of hydrogen storage intermetallic compounds $RECo_5$ (RE=Nd, Ho, Er and Tm) was studied with the aim to obtain theoretical information about their physical and chemical properties. Standard calculation methods within DFT (density functional theory) were used, whereby the corresponding approaches LSDA and LSDA+U (local spin density approximation) were employed. Magnetic moments and relative stabilities of ferrimagnetic and ferromagnetic ordering of 4*f* and 3*d* spin sublattices were calculated. It was found that LSDA gives poor results regarding 4*f* magnetic moments and the type of the magnetic order in the ground state. However, LSDA+U considerably improves the description of the relative stabilities of the ferrimagnetic and ferromagnetic sublattices (Miletić and Blažina, 2009). It was also found that the theoretically obtained values are in good agreement with the experimental data.

New paramagnetic hexanuclear clusters of tantalum

The new cluster $[Et_4N][Ta_6Br_{12}(H_2O)_6]Br_4 \cdot 4H_2O$ crystallizes in the tetragonal $I4_1/a$ space group and contains discrete $[Ta_6Br_{12}(H_2O)_6]^{3+}$ cations with the octahedron of metal atoms edge-bridged by bromine atoms and with water molecules occupying all

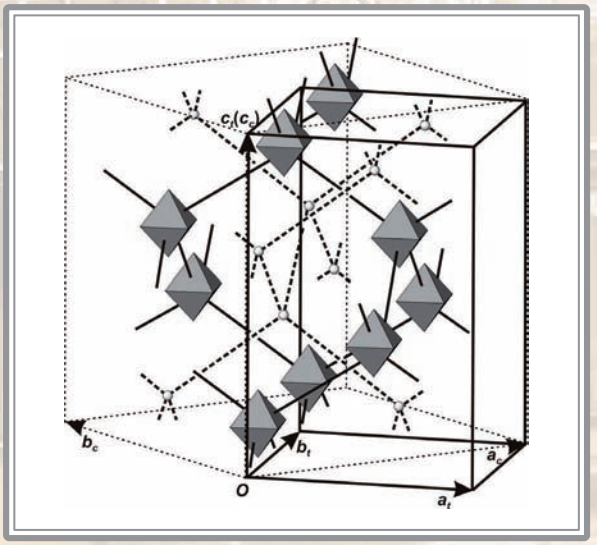


Figure 4. Two interpenetrating (pseudo)diamond nets formed by the paramagnetic $[Ta_6Br_{12}(H_2O)_6]^{3+}$ (octahedra) and diamagnetic $[Et_4N]^+$ (spheres) cations.

six terminal positions. The present four-fold inversion crystallographic symmetry gives rise to the emanation of the three-dimensional (pseudo)diamond lattices formed by the paramagnetic $[Ta_6Br_{12}(H_2O)_6]^{3+}$ entities and the diamagnetic $[Et_4N]_+$ cations (Figure 4). The nearest neighbouring cluster units create short intermolecular contacts across the bridging bromine atoms, which might have a special role in the expected intercluster magnetic exchange interactions (Perić et al., 2009).

Physico-chemical effects of ionizing radiations in materials

The experience accumulated during the long-standing co-operation of the Radiation Chemistry and Dosimetry Laboratory with the Croatian Conservation Institute, Academy of Fine Arts of the University of Zagreb and a number of museums, galleries and archives throughout Croatia on the application of irradiation techniques for the preservation of cultural and artistic heritage objects of organic origin has been acknowledged in an open publication for the first time.

Subcellular biochemical and phylogenetic diversity of aquatic organisms

Using novel machine learning techniques, the authors determined and discriminated blood biochemical parameters between three aquaculture-influenced marine fish species based on machine learning methods. This is the first time that these classification algorithms were used as a framework for rapid differentiation between three fish species (Čož-Rakovac et al., 2009).

PATENTS

HR patent: 1844674073709551615. Subotić B, Kosanović C, Bosnar S, Antonić Jelić T, Bronić J. Zeolite 4A with new morphological properties, their synthesis and use.

NEW EQUIPMENT

A **FT-IR spectrometer**, model ALPHA-T, Bruker Optics, a precise and very practical, portable laboratory instrument, was purchased by the support of Ministry of Science, Education and Sports.

A CombiFlash Rf **flash chromatography system**, with high-productivity automation, UV detection and peak separation, was purchased through the UKF project (Organometallic and inorganic bioconjugates as potential enantioselective catalysts).

The acquisition of a **Harshaw 6600 thermoluminescent dosimetry reader** was assisted by the Ministry of Science, Education and Sports providing 50% of the cost.

EDUCATION

Scientists from the Division contributed to 18 undergraduate and postgraduate courses in 2009 as part of the involvement in the educational program of Universities in Zagreb, Osijek and Dubrovnik.

AWARDS

1. Damir Kralj: Procedure for preparation of precipitated calcium carbonate by semi-continuous process, Silver ARCA at The 7th International fair of inventions, new ideas, products and technologies, Zagreb, 2009
2. Marko Ukrainczyk: The Award of the Croatian Society of Chemical Engineers for Young Chemical Engineers, April 22, 2009.

PROJECTS

Projects supported by the Ministry of Science, Education and Sport

1. Synthesis and microstructure of metal oxides and oxide glasses, Svetozar Musić
2. Study of influence of aluminosilicate precursors on their transformations, 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 radiations in materials, Dušan Ražem
8. Subcellular biochemical and phylogenetic diversity of aquatic organisms, Rozelindra Čož-Rakovac

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

1. New functional materials, Svetozar Musić

Research, developmental and international projects

1. Metal oxides: structural and magnetic properties, Mira Ristić (Croatian-Serbian Scientific Cooperation Programme for 2008-2010).
2. Optimization of the synthesis process of zeolite A with special emphasis on the control of particulate properties (size and shape of zeolite A crystals), Boris Subotić (Bartex-Bartol and Ruđer Bošković Institute co-operation scientific research – 2nd phase).
3. Atomic-force microscopy study of the crystallization of zeolites A, X and silicalite from amorphous (alumino)silicates, Cleo Kosanović (Croatian-Hungarian Intergovernmental Science and Technology Cooperation Programme 2007-2009).
4. Study of the processes of formation and growth of zeolite nuclei in the matrix of amorphous aluminosilicate gel, Josip Bronić (COGITO, Croatian-French bilateral project 2009-2010).
5. Physical-structural studies of mixed-halide metal-atom clusters building blocks, Berislav Perić (Croatian-French Program "Cogito", Hubert Curien Partnership 2009/2010).
6. Organometallic and inorganic bioconjugates as potential enantioselective catalysts, Srećko Kirin (UKF project, 2009/2010).
7. Free Radicals in Chemical Biology (CHEMBIORADICAL), Branka Mihaljević (COST Action Project number CM0603).
8. Solid state dosimetry systems for various dosimetry fields, Maria Ranogajec-Komor, (Bilateral scientific and technical co-operation between Croatian Academy of Sciences and Arts and Hungarian Academy of Science, 2007-2009).
9. Characterization, intercomparison and application of radiophotoluminescence (RPL) dosimetry system according to international standards and protocols, Maria Ranogajec-Komor (Scientific co-operation between Ruđer Bošković Institute and Chiyoda Technology Corporation, Japan).
10. Solid state detectors in mixed radiation fields dosimetry, Saveta Miljanić (Croatian- Hungarian Intergovernmental Scientific and Technical Cooperation, 2009-2010).
11. Radiation protection in medicine: The risk of early and late health effects from the use of radiation therapy, Saveta Miljanić (EURADOS Working Group 9).
12. Enhancing quality control methods and procedures for radiation technology, Dušan Ražem (International Atomic Energy Agency Regional Technical Co-operation Project; Project number: RER 8/017).
13. Nuclear techniques for the characterisation and preservation of cultural heritage artefacts in the Europe Region, Branka Katušin-Ražem (International Atomic Energy Agency Regional Technical Co-operation Project; Project number: RER 8/015).
14. Environmental dose measurements using TL dosimeters, Branko Vekić, Maria Ranogajec-Komor, Željka Knežević (Contract with NPP Krško).
15. Preservation of oyster production by asserting its autochthony, Ivančica Strunjak-Perović *(Ministry of Agriculture,* Fisheries and Rural Development, VIII-5-50/08).
16. Breeding and Selection in Aquaculture – Gacka d.o.o., Natalija Topić Popović (Scientific and technological research project,

Ministry of Agriculture, Fisheries and Rural Development, 324-01/08-01/393).

17. Determination of genetic structure and restoration of autochthonous population of brown trout in the National Park Plitvice Lakes, Rozelindra Čož-Rakovac (National Park Plitvice Lakes/ Ministry of Environmental Protection, Physical Planning and Construction, 21320/06).
18. Breeding and Selection in Aquaculture, Fishery 1961 d.o.o., Ivančica Strunjak-Perović (Scientific and technological research project, *Ministry of Agriculture,* Fisheries and Rural Development, 324-01/08-01/401).
19. Applications of new technologies in shellfish production, Mateo Milković, co-investigator Rozelindra Čož-Rakovac, (Scientific and technological research project, Croatian Institute of Technology)
20. Aquatic animal health monitoring, Rozelindra Čož-Rakovac (contracts with 9 international and national companies).

SELECTED INVITED LECTURES

1. Ristić M. Nanostructured metal oxides – synthesis and characterization. Croatian-Japanese Workshop on Materials Science, Zagreb, Croatia, June 29-30, 2009.
2. Kosanović C. Thermal transformations of amorphous aluminosilicate precursors to ceramics. The Second Croatian-Slovenian Symposium on Zeolites. Ljubljana (Slovenia), October 1-2, 2009.
3. Planinić P. Transition metal complexes as the basis for new materials: Synthesis, structures and properties. Croatian-Japanese Workshop on Materials Science, Zagreb, Croatia, June 29-30, 2009.
4. Ranogajec-Komor M. Solid state passive dosimeters and their applications. Fu Dan University, Institute of Radiation Medicine, Shanghai, China, November 26, 2009.
5. Knežević Ž, Miljanić S, Milković Đ, Ranogajec-Komor M. Overview of RPL investigations at the Ruđer Bošković Institute. 5th International Workshop on Individual Monitoring, Oarai, Japan, December 1-2, 2009.
6. Jadan M. Genetic analyses of freshwater crayfish. 6th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, July 1, 2009.

SELECTED ORGANIZED CONFERENCES

The Second Croatian-Slovenian Symposium on Zeolites, Ljubljana (Slovenia) 01 - 02. 10. 2009. Organization: Croatian Zeolite Association, Ruđer Bošković Institute and Slovenian Chemical Society. President of the Organizing Committee: Josip Bronić (Ruđer Bošković Institute).

SELECTED PUBLICATIONS

1. Žic M, Ristić M, Musić S: Precipitation of α-Fe_2O_3 from dense α-FeOOH suspensions with added ammonium amidosulfonate. *J Mol Struct* **924–926** (2009), 235-242.
2. Gotić M, Koščec G, Musić S: Study of the reduction and reoxidation of substoichiometric magnetite. *J Mol Struct* **924-926** (2009), 347.
3. Kosanović C, Havenscak K, Subotić B, Svetličić V, Mišić T, Cziraki T, Huhn G: A Contribution to Understanding the Mechanism of Crystallization of Silicalite-1 in Heterogeneous Systems (Hydrogels). *Micropor Mesopor Mat* **123** (2009), 150.
4. Njegić Džakula B, Brečević Lj, Falini G, Kralj D: Calcite crystal growth kinetics in the presence of charged synthetic polypeptides. *Cryst Growth Des* **9 (5)** (2009), 2425-2434.
5. Ukrainczyk M, Kontrec J, Kralj D: Precipitation of different calcite crystal morphologies in the presence of sodium stearate. *J Coll Int Sci* **329** (2009), 89.
6. Miletić GI, Blažina Ž: Magnetic order in $ErCo_5$ and $TmCo_5$ from the electronic structure calculations. *J Magn Magn Mater* **321** (2009), 2300.
7. Miletić GI, Blažina Ž: Magnetic properties of $NdCo_5$ and $HoCo_5$ from the electronic structure calculations. *J Magn Magn Mater* **321** (2009), 3888.

8. Perić B, Jozić D, Planinić P, Brničević N, Giester G: Synthesis and characterization of $[Et_4N][Ta_6Br_{12}(H_2O)_6]Br_4 \cdot 4H_2O$ (Et = ethyl), a new compound with the paramagnetic $[Ta_6Br_{12}(H_2O)_6]^{3+}$ cluster core. *J Solid State Chem* **182** (2009), 2443.
9. Katušin-Ražem B, Ražem D, Braun M: Irradiation treatment for the protection and conservation of cultural heritage artefacts in Croatia. *Radiat Phys Chem* **78** (2009), 729.
10. Milković Đ, Garaj-Vrhovac V, Ranogajec-Komor M, Miljanić S, Gajski G, Knežević Ž, Beck N: Primary DNA damage assessed with the comet assay and comparison to the absorbed dose of diagnostic X-rays in children. *Internat J Toxicol* **28** (2009), 405.
11. Čož-Rakovac R: Classification accuracy of algorithms for blood chemistry data of three aquaculture-influenced marine fish species. *Fish Phys Biochem* **35** (2009), 641.
12. Strunjak-Perović I, Topić Popović N, Čož-Rakovac R, Jadan M: Nuclear abnormalities of marine fish erythrocyte. *J Fish Biol* **74** (2009), 2239.

Division of Molecular Biology

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

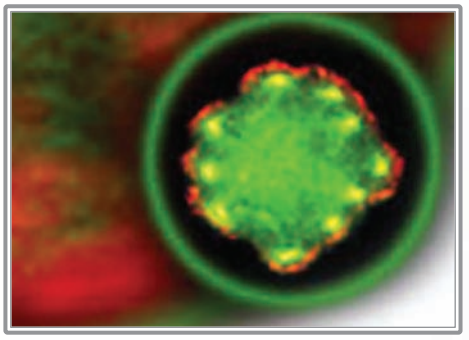
ZMB

DIVISIONAL ORGANISATION

Head: Igor Weber

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

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



OVERVIEW OF THE DIVISION

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

In 2009, members of the Division of molecular biology participated in the teaching of more than 30 undergraduate and postgraduate courses at Croatian universities. During that year they also supervised more than 20 diploma, MSc, and PhD theses. A series of practical courses in biology and medicine was organized in our Division by Andreja Ambriović Ristov (http://www.tecajevi-irb.com).

TOP ACHIEVEMENTS

Efficiency of photosynthetic energy conversion

Working in tandem, two photosystems in the chloroplast thylakoid membranes produce a linear electron flow from H_2O to $NADP^+$. Final electron transfer from ferredoxin to $NADP^+$ is accomplished by a flavoenzyme ferredoxin: $NADP^+$ oxidoreductase (FNR). We describe the rhodanase-like protein (TROL) of plant photosynthetic membranes which docks FNR and enables efficient photosynthesis. *Arabidopsis* TROL knock-out plants have decreased linear electron flow and increased photooxidative tolerance. Alterations in nuclear gene expression indicate the existence of a novel metabolic retrograde signaling pathway (Jurić et al., 2009).

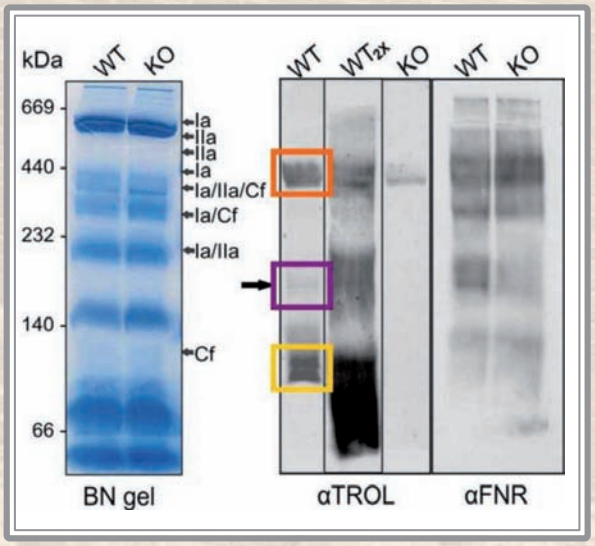


Figure 1. Supramolecular complexes of TROL in photosynthetic membranes.

Cisplatin sensitivity related to late DNA damage processing

We performed a comparative study using a pair of isogenic Chinese hamster cells differing in their sensitiviy to cisplatin. CL-V5B cells were hypersensitive to the killing effect of this drug as compared to wild-tpye V79wt cells, although the initial DNA adduct formation was reduced in CL-V5B cells. Our study provides shows that the initial level of cisplatin-DNA adducts and the corresponding early DNA damage response do not necessarily predict the outcome of cisplatin treatment. Rather, the accuracy of DNA damage processing and late checkpoint control mechanisms determine the extent of cell death triggered by cisplatin-induced DNA lesions (Brozović et al., 2009).

Roles of ExoI and SbcCD nucleases in "reckless" DNA degradation in *Escherichia coli*

Exponentially growing *recA* mutant cells of *E. coli* display pronounced DNA degradation that starts at the sites of DNA damage, and depends on the RecBCD nuclease (ExoV) activity. As a consequence of this "reckless" DNA degradation, populations of *recA* mutants contain a large proportion of anucleate cells. We have found that con-

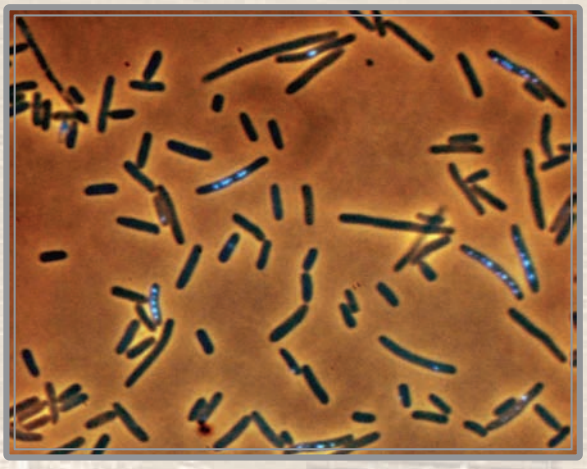


Figure 2. Anucleate cells as a consequence of "reckless" DNA degradation in UV-irradiated E. coli recA mutants.

comitant inactivation of ExoI and SbcCD nucleases (by mutations in *xonA* and *sbcD* genes) strongly suppresses both DNA degradation and anucleate cell production in normally grown as well as in UV-irradiated, *recA* cells. Our results suggest that the role of ExoI and SbcCD might be in blunting DNA ends thereby producing suitable substrates for RecBCD binding (Zahradka et al., 2009).

Satellite DNAs as phylogenetic markers

Satellite DNAs (DNA sequences repeated in tandem) are landmarks of heterochromatic chromosomal portions. They are characterized by rapid genomic turnover, achieved mostly by copy-number alterations of families in a genome (the library model). This evolutionary pathway frequently obscures sequence comparisons among species, making satellite DNA sequences an unreliable phylogenetic marker. We used the presence/absence of satellite families in a library as a character to reconstruct phylogeny of examined root-knot species. In this work, it was shown for the first time that the presence/absence of satellite DNAs in the library can be used as a phylogenetic marker (Meštrović et al., 2009).

Centromere: Structure and Evolution

The centromere is a chromosomal locus that regulates the proper pairing and segregation of the chromosomes during cell division. Despite their conserved, essential function, centromeres are characterized by the rapid evolution of both centromeric DNA and proteins. The book Centromere: Structure and Evolution presents current views on centromere structure and identity. It deals with the epigenetic concept of centromere establishment and maintenance as well as with the role of DNA and centromeric transcripts in centromere formation and function. Special emphasis is placed on centromere evolution: different evolutionary models are discussed in detail and the latest research on the evolution of new centromeres and neocentromeres is presented. Written by world reknowned specialists in the field this book represents the most up-to-date findings on the study of centromeres (Ugarković, ed. 2009).

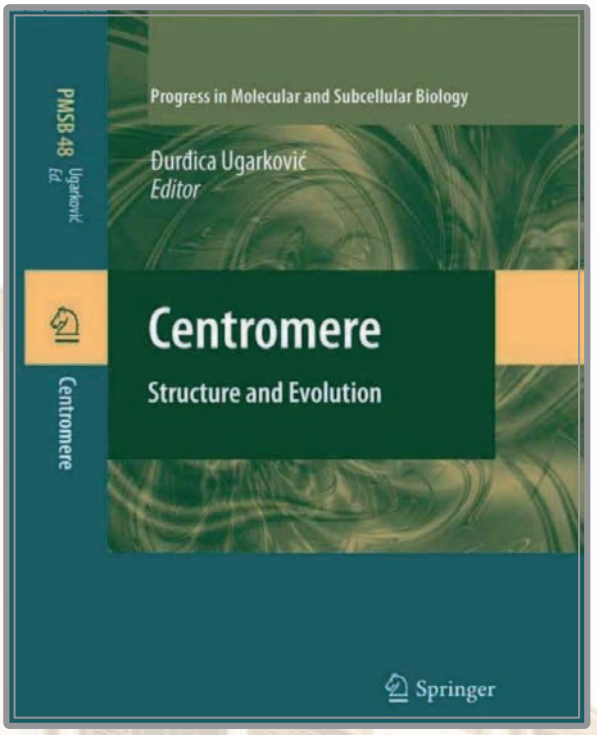


Figure 3. Centromere: Structure and Evolution, Progress in Molecular and Subcellular Biology, Vol. 48, 2009, Springer Verlag. Editor: Đurđica Ugarković.

MODERN FACILITIES, METHODS AND EQUIPMENT

Centre for DNA sequencing

The DNA centre for DNA sequencing, under the supervision of Helena Ćetković as part of the Laboratory for Molecular Genetics, continued to provide services during 2009. Besides DNA sequence analyses, it also offers a microsatellite genotyping method for external users. More than 2500 sequence analyses were performed in this year at the DNA centre using an ABI-Prism 3100 Sequencer.

Confocal laser scanning microscope

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

AWARDS

Željka Pezer received the Željko Trgovčević Award for year 2008. This award is granted by Croatian Genetical Society and RBI - Department of Molecular Biology for research excellence shown by young researchers in molecular biology. Željka Pezer was awarded the prize for her comprehensive study of transcription of satellite DNAs published in PLoS ONE, Seminars in Cancer Biology and Cytogenetics and Genome Research.

Mariastefania Antica received the Annual Award from the Croatian Immunological Society, which honours the best scientific paper in immunology published by a member of the Society in the past year (2008).

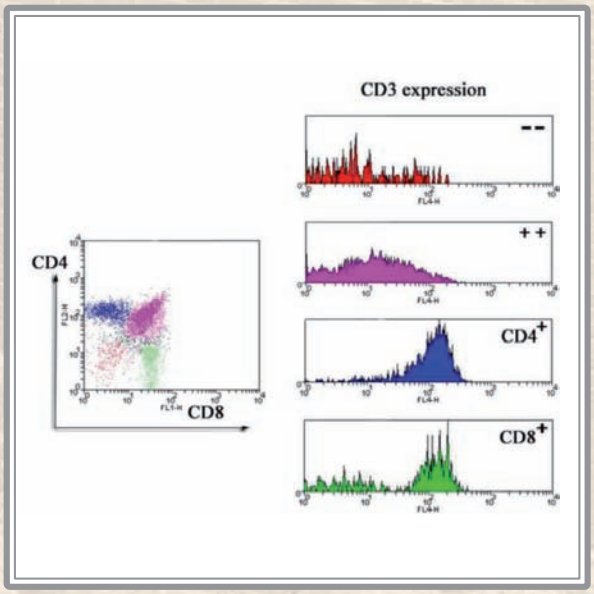


Figure 4. Expression of CD3, CD4 and CD8 proteins in rat thymus cell subpopulations.

EDUCATION

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

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

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

Program supported by the Ministry of Science, Education and Sports

1. Molecular fundaments of biological processes, Miroslav Plohl.

OTHER PROJECTS

1. Structural and functional analysis of noncoding heterochromatic DNA in insect *Tribolium castaneum*, Đurđica Ugarković, (EC FP6 Marie Curie Host Fellowship for Transfer of Knowledge project MTKD-CT-2006-042248)
2. Biophotonics approach to regulation of the actin cytoskeleton dynamics by small GTPase proteins, Igor Weber (UKF 1A Grant Agreement 9/07)
3. Phylostratigraphic analysis of disease genes expression in the context of life cycle, Tomislav Domazet-Lošo (UKF Young Researchers Grant 3A)
4. Transcriptional regulation in human leukemic cells, Mariastefania Antica (MZOŠ, bilateral project with Austria, 910-08/07-01/00129)
5. Subcellular localization of glutathione and cysteine in cyanobacteria, Hrvoje Fulgosi (MZOŠ, bilateral project with Austria, 910-08/07-01/00125)
6. Study of DNA, protein components and their interactions in holocentric chromosomes of root-knot nematodes of the genus *Meloidogyne*, Miroslav Plohl (MZOŠ, Cogito bilateral projet with France, 910-08/06-01/00093)
7. Analysis of cytoskeleton dynamics during phagocytosis and cell migration, Igor Weber (MZOŠ, DAAD bilateral project with Germany, 910-08/07-01/00143)
8. Molecular mechanisms determining cellular susceptibility to platinum drugs, Maja Osmak (MZOŠ, DAAD bilateral project with Germany, 910-08/07-01/00145)
9. Origin and evolution of satellite DNAs in two economically relevant *Venerupis* bivalve molluscs of the Adriatic Sea, Miroslav Plohl (MZOŠ, MSES bilateral project with Italy)
10. Plant hormones in development and biotic stress using biochemical and molecular approaches, Branka Salopek-Sondi (MZOŠ, bilateral project with Slovenia, 919-08/06-01/00208)
11. Diaryrtriazens: a new group of potential anticancer drugs. Maja Osmak (MZOŠ, bilateral project with Slovenia, 910-08/08-01/00312)
12. Regeneration of articular cartilage of the knee, Andreja Ambriović Ristov (MZOŠ, HITRA–TEST, 381-01/06-02/00032)
13. Construction, development and application of target vectors, Ivica Rubelj (Croatian Institute of Technology)
14. Dedifferentiation of committed stem cells in leukemia, Mariastefania Antica (Croatian Academy of Sciences and Arts – HAZU)
15. Improving the quality of products based on sour cherry maraska juice, Helena Ćetković (Maraška Ltd., MPŠVG, 24-14/07)

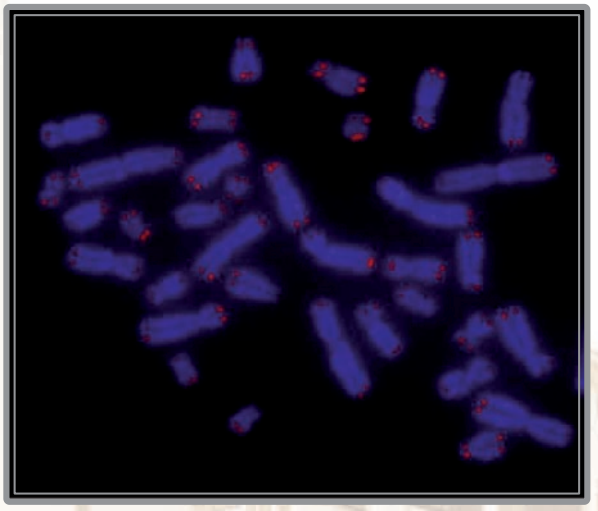


Figure 5. Human chromosomes stained with DAPI (blue); telomeres visualized with Cy3 PNA-FISH (red).

SELECTED INVITED LECTURES

1. Jernej B, Čičin-Šain L: Wistar-Zagreb 5HT rats: a rodent model with constitutional up-regulation/downregulation of serotonin transporter. 12th Multidisciplinary International Neuroscience and Biological Psychiatry Conference “Stress and Behavior”. St. Petersburg, Russia, May 16-20, 2009.
2. Bielen A, Abramić M, Pigac J, Vujaklija D: The SGNH-lipolytic enzymes in *Streptomyces*

species. Biology of *Streptomycetes*, Münster, Germany, October 7 – 11, 2009.
3. Filić V: Fluorescent probes illuminate role of Rac1A in regulation of the actin cytoskeleton in *D. discoideum*. 9th Multinational Conference on Microscopy. Graz, Austria, August 30 – September 4 2009.
4. Weber I: Monitoring the dynamics of Rac proteins in *Dictyostelium discoideum*. EMBO Conference on Physics of Cells: From the Edge to the Heart. Primošten, Croatia, September 6-13, 2009.
5. Vujaklija D, Bielen A, Abramić M, Pigac J: The SGNH-hydrolase from Streptomycetes. 10th Croatian Biological Congress, Osijek, Croatia, September 14-20, 2009.
6. Harcet M, Ćetković H, Perina D, Müller W, Vlahoviček K: Comparative genomics reveals broad genetic repertoire of simplest metazoans – sponges (Porifera). 10th Croatian Biological Congress, Osijek, Croatia, September 14-20, 2009.
7. Plohl M, Mravinac B, Meštrović N: Dual character in satellite DNA evolution: rapid changes vs. nucleotide sequence persistence. 10th Croatian Biological Congress, Osijek, September 14-20, 2009.
8. Harcet M: Sponges as model organisms in studies of evolution. Scientific Symposium "Darwin 200", Zagreb, Croatia, December 11, 2009.
9. Plohl M: Changes and persistence in the evolution of satellite DNAs. Scientific Symposium "Darwin 200", Zagreb, Croatia, December 11, 2009.
10. Mravinac B: Evolution of satellite DNAs – the sense of „nonsense". Scientific Symposium "Darwin 200", Zagreb, Croatia, December 11, 2009.
11. Rubelj I: Evolution, telomeres and genome stability. Scientific Symposium "Darwin 200", Zagreb, Croatia, December 11, 2009.

SELECTED ORGANIZED CONFERENCES

1. 10th Croatian Biological Congress, Osijek, Croatia, September 14-20, 2009 (M. Plohl)
2. 10th International School on Biophysics, Rovinj, Croatia, September 15-30, 2009 (I. Weber and K. Zahradka).

SELECTED PUBLICATIONS

Research articles

1. Jurić S, Hazler-Pilepić K, Tomašić A, Lepeduš H, Jeličić B, Puthiyaveetil S, Bionda T, Vojta L, Allen JF, Schleiff E, Fulgosi H: Tethering of ferredoxin:$NADP^+$ oxidoreductase to thylakoid membranes is mediated by novel chloroplast protein TROL. *Plant J* **60** (2009), 783.
2. Meštrović N, Plohl M, Castagnone-Sereno P: Relevance of satellite DNA genomic distribution in phylogenetic analysis: A case study with root-knot nematodes of the genus *Meloidogyne*. *Mol Phylogenet Evol* **50** (2009), 204.
3. Zahradka K, Buljubašić M, Petranović, M, Zahradka D: Roles of ExoI and SbcCD nucleases in "reckless" DNA degradation in *recA* mutants of *Escherichia coli*. *J Bacteriol* **191** (2009), 1677.
4. Klarica M, Orešković D, Božić B, Vukić M, Butković V, Bulat M: New experimental model of acute aqueductal blockage in cats: effects on cerebrospinal fluid pressure and the size of brain ventricles. *Neuroscience* **158** (2009), 1397.

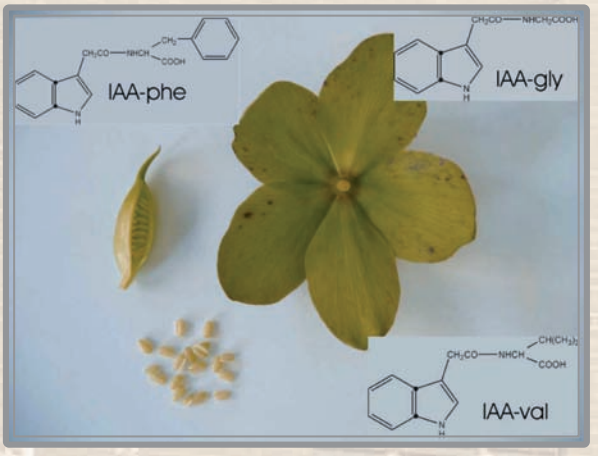


Figure 6. The auxin (indole-3-acetic acid, IAA) conjugates with amino acids Gly, Phe and Val were identified in the Christmas rose (Helleborus niger L.) seeds.

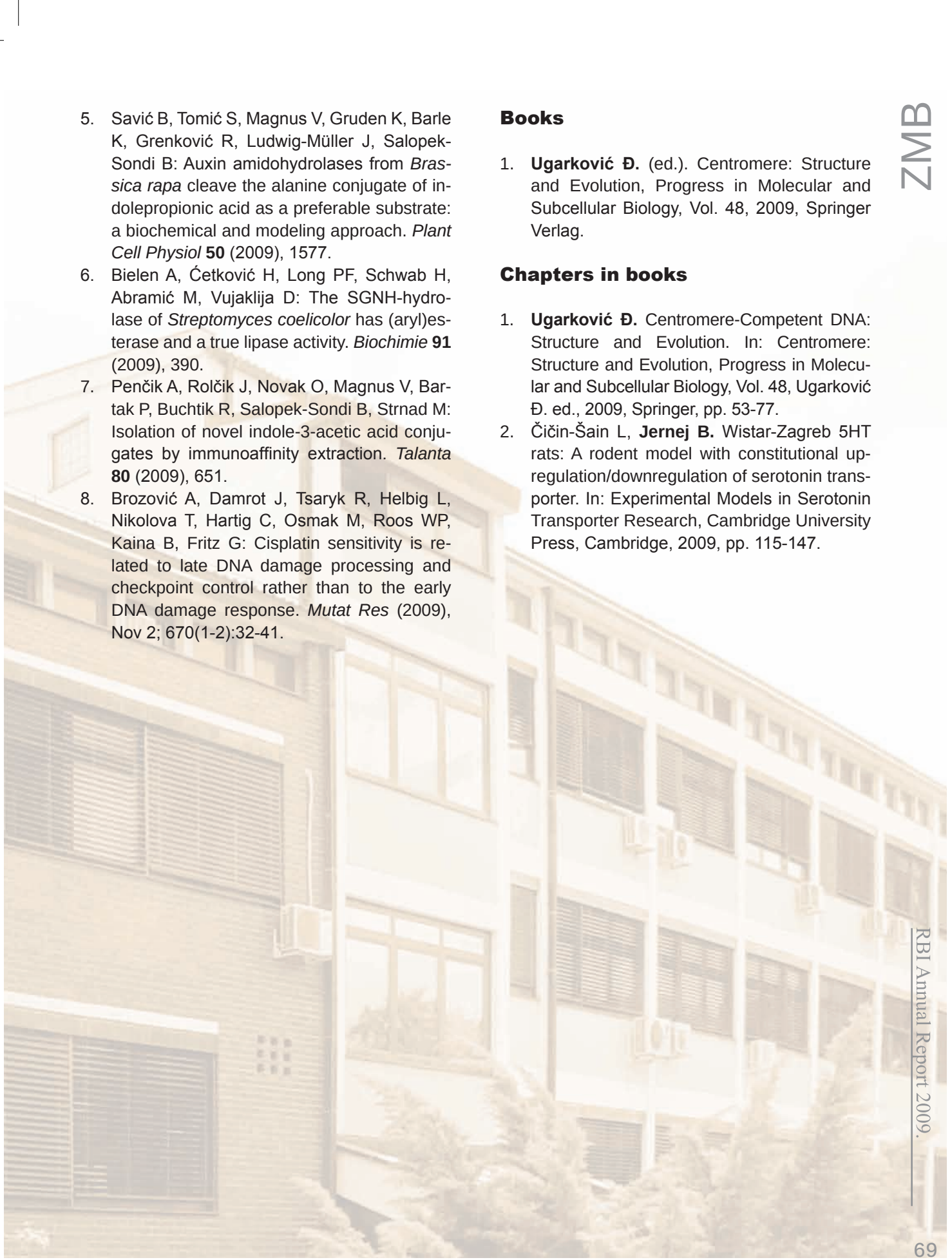
5. Savić B, Tomić S, Magnus V, Gruden K, Barle K, Grenković R, Ludwig-Müller J, Salopek-Sondi B: Auxin amidohydrolases from *Brassica rapa* cleave the alanine conjugate of indolepropionic acid as a preferable substrate: a biochemical and modeling approach. *Plant Cell Physiol* **50** (2009), 1577.
6. Bielen A, Ćetković H, Long PF, Schwab H, Abramić M, Vujaklija D: The SGNH-hydrolase of *Streptomyces coelicolor* has (aryl)esterase and a true lipase activity. *Biochimie* **91** (2009), 390.
7. Penčik A, Rolčik J, Novak O, Magnus V, Bartak P, Buchtik R, Salopek-Sondi B, Strnad M: Isolation of novel indole-3-acetic acid conjugates by immunoaffinity extraction. *Talanta* **80** (2009), 651.
8. Brozović A, Damrot J, Tsaryk R, Helbig L, Nikolova T, Hartig C, Osmak M, Roos WP, Kaina B, Fritz G: Cisplatin sensitivity is related to late DNA damage processing and checkpoint control rather than to the early DNA damage response. *Mutat Res* (2009), Nov 2; 670(1-2):32-41.

Books

1. **Ugarković Đ.** (ed.). Centromere: Structure and Evolution, Progress in Molecular and Subcellular Biology, Vol. 48, 2009, Springer Verlag.

Chapters in books

1. **Ugarković Đ.** Centromere-Competent DNA: Structure and Evolution. In: Centromere: Structure and Evolution, Progress in Molecular and Subcellular Biology, Vol. 48, Ugarković Đ. ed., 2009, Springer, pp. 53-77.
2. Čičin-Šain L, **Jernej B.** Wistar-Zagreb 5HT rats: A rodent model with constitutional upregulation/downregulation of serotonin transporter. In: Experimental Models in Serotonin Transporter Research, Cambridge University Press, Cambridge, 2009, pp. 115-147.



Division of Molecular Medicine

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

ZMM

DIVISIONAL ORGANIZATION

Head: Tatjana Marotti

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 Epigenomics, Koraljka Gall-Trošelj
- Laboratory of Molecular Virology and Bacteriology, Magdalena Grce
- Laboratory of Molecular Endocrinology and Transplantation, Mirko Hadžija
- Laboratory for Personal Medicine, Sanja Kapitanović
- Laboratory of Functional Genomics, Marijeta Kralj
- Laboratory for Hereditary Cancer, Sonja Levanat
- Laboratory for reactive radicals, Tatjana Marotti
- Laboratory of Molecular Neuropsychiatry, Dorotea Muck-Šeler
- Laboratory of Molecular Oncology, Jasminka Pavelić
- Laboratory of Molecular Neuropharmacology, Silva Hečimović
- Translational Medicine Laboratory, Oliver Vugrek
- Laboratory for Oxidative Stress, Neven Žarković
- Animal Quarters, Ranko Stojković

OVERVIEW OF THE DIVISION

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

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

Members of the division provided significant contributions to higher education by providing numerous courses at the undergraduate and graduate level in Zagreb, Split,

Osijek, Rijeka, Dubrovnik and Zadar. During 2009, members of DMM led 47 courses in Ph.D. studies, and they supervised 50 B.Sc. theses, 15 M.Sc. theses and 17 Ph.D. theses.

TOP ACHIEVEMENTS IN BASIC AND APPLIED RESEARCH

Multidrug resistance/P-glycoprotein and insulin degrading enzyme

We have found evidence in human tumor cell lines for complex formation between the multidrug resistance/P-glycoprotein (MDR1/P-gp) and the insulin degrading enzyme (IDE). These results are consistent with a recently elaborated putative tumor suppressor role of IDE that is possibly counteracted by the MDR1/P-pg through the displacement of intracellular growth stimulators such as insulin and/or nuclear factor kappa-B from their IDE binding sites. Our work constitutes the first experimental demonstration of the anticipated MDR1-IDE heterodomer, which thus provides a lead for significantly expanding current efforts to further understand and modulate MDR (Radulescu et al., 2009).

Proteomic profiling of palmar fasciae tissues from Dupuytren's disease

We have reported for the first time the proteomic profiling of diseased versus unaffected patient-matched palmar fasciae tissues from Dupuytren's disease patients using 2D PAGE coupled with mass spectrometry analysis. The identified proteins was then used to create a protein-protein interaction network (interactome). Such an integrated approach revealed the involvement of several different molecular processes related to Dupuytren's disease progression, including extra- and intra-cellular signalling, oxidative stress, cytoskeletal changes, and alterations in cellular metabolism (Pavelić Kraljević et al., 2009).

Complex role of an iron compound on the immune and inflammatory response

The time-dependent immuno-modulatory effects of an iron (Fe^{3+}) compound iron polyisomaltosate, on serum iron, interleukin-6, serotonin concentration, neutrophil activity, and NF-κB activation in peritoneal macrophages and spleen cells in rats was shown. These effects might be achieved via induction of the intracellular signalling pathway for NF-κB activation in peritoneal macrophages and later in spleen cells, together with increases of serum serotonin and interleukin-6. Iron polyisomaltosate presumably activated reactive oxygen species, which stimulated the acute phase reactants in the liver (Poljak-Blaži et al., 2009).

Development of tolerance during chronic treatment of diazepam and zolpidem

The effects of acute and repeated administration of diazepam and zolpidem were tested to compare their sedative and anticonvulsant properties, and to evaluate the importance of GABA-A receptor subunits for development of tolerance during chronic treatment. Our study showed good anticonvulsant potency of zolpidem. The results indicate development of tolerance to effects of diazepam and zolpidem, and suggested that α5-containing GABA-A receptors are not crucial for the development of sedative and anticonvulsant tolerance (Vlainić and Peričić, 2009).

Rosacea

Rosacea is a common chronic inflammatory dermatosis of unknown etiology, characterized by various combinations of cutaneous signs such as flushing, erythema, telangiectasia, edema, papules, papulopustules, ocular lesions and phymas. We have shown for the first time that significantly

higher serum peroxide levels and significantly lower serum total antioxidative potential levels exist in rosacea patients as compared with healthy control subjects. The number of ferritin positive cells was significantly higher in skin samples of rosacea patients than in control samples, and the number of ferritin positive cells was significantly higher in skin of patients with severe stage of disease. The differences in the expression of ferritin, the higher peroxide levels and lower antioxidative potential, supported the hypothesis that rosacea is a systemic oxidative stress disease (Sredoja Tisma et al., 2009).

Dietary exposure to aristolochic acid is a major risk factor for endemic nephropathy

Aristolochic acid (AA), an established nephrotoxin and human carcinogen found in all *Aristolochia* species (Figure 1), preferentially binds to purines in DNA and is associated with a high frequency of A → T transversions in the p53 gene. We reported the presence of AA-DNA adducts in renal cortex and A → T mutations in tumor tissue of patients from Croatia and Bosnia with endemic (Balkan) nephropathy. These data support the hypothesis that dietary exposure to AA is a major risk factor for this devastating chronic renal disease (Slade et al., 2009).

Figure 1. Aristolochia clematitis growing in the middle of wheat field in the Croatian endemic village of Kaniža during harvest time 2008.

The role of *nm23-H1* in CAL 27 oral carcinoma cells

Our recent data on the role of *nm23-H1* show that CAL 27 oral carcinoma cells overexpressing this gene exhibit reduced migratory and invasive potential, and adhere more strongly to components of the extracellular matrix. Although the mechanism of this phenomenon is still under investigation, we expect *nm23-H1* to be a true metastasis suppressor gene/protein in oral squamous cell carcinoma (Bago et al., 2009)

TOP ACHIEVEMENTS IN APPLIED RESEARCH

Protection from cervical cancer

Cervical cancer incidence and mortality rates have been reduced substantially in those countries that have effectively organized screening programs. However, cervical screening is generally inefficient and unworkable in many regions of the world where the appropriate infrastructure is missing. Therefore, prophylactic vaccination against the major cause of cervical cancer, the carcinogenic human papillomavirus (HPV) types 16 and 18, represents an alternative for cervical cancer control. Together, primary and secondary prevention, i.e. HPV vaccination and cervical screening offer maximal protection from cervical cancer (Grce 2009; Nicula et al., 2009).

Novel potential anticancer compounds

During 2009 about 100 newly synthesized compounds were screened *in vitro* for potential antitumor activity and the possible mechanisms of action were ascertained for the most effective ones (Figure 2). Of special significance is a study that presents novel imidazolinyl-substituted benzothiophene derivatives as potential anticancer

drugs. The molecular mechanisms of antitumor actions were analyzed by comparing structure, DNA interactions, and biological effects of tested compounds. Biological analyses involving cell cycle analysis, proliferation assay, topoisomerase assay and immunofluorescence revealed that the tested compounds possess high chemotherapeutic potential. The most intriguing result is the observation that only a minor structural difference between derivatives results in a major difference in their targets/mechanisms of action (DNA and tubulin disruption) (Ester et al., 2009).

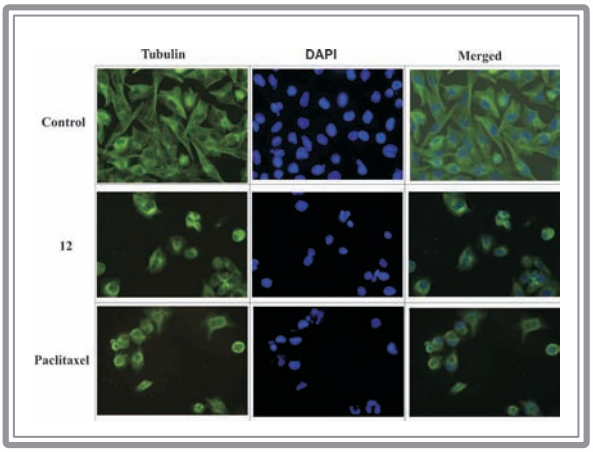


Figure 2. Tubulin immunofluorescence staining of MiaPaCa-2 cells. Coverslips containing MiaPaCa-2 cells were incubated with compound 12 (5 μM) and Paclitaxel (1nM) for 24 hours, and stained with anti-alpha-tubulin antibody, FITC-conjugated secondary antibody, and DAPI.

The first lethal case of S-Adenosylhomocysteine hydrolase (AHCY) deficiency

We have described the first lethal case of S-Adenosylhomocysteine hydrolase (AHCY) deficiency. We have identified two allelic pointmutations in the AHCY gene that are related to the death of a female infant. Using recombinant DNA technology, we performed functional analysis of both mutations and confirmed loss of enzymatic activity of mutated AHCY protein (Vugrek et al., 2009).

INTERNATIONAL FUNCTIONS

Dorotea Muck-Šeler was appointed a member of the Editorial Board of the international journal cited in Current Contents, Progress in Neuro-Psychopharmacology & Biological Psychiatry. This appointment was awarded for her long time role as a reviewer for this journal.

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

DOMESTIC FUNCTIONS

Tatjana Marotti was appointed director of the Division of Molecular Medicine at Ruđer Bošković Institute.

AWARDS

The Annual Croatian State Award for Science

Award to Nela Pivac: The Croatian State Award, the most prestigious scientific recognition available in Croatia, was given to Nela Pivac, senior scientist at the Division of Molecular Medicine. Nela Pivac was given the award for her research in the field of biomedicine, especially her significant achievements in research studying the molecular basis and treatment of psychiatric disorders.

Best poster award at the FEBS

Martina Malnar received the best poster award at the FEBS advanced course “Lipid signalling and diseases” in Ortona, Italy, September 9-15, 2009.

Patent application

Kralj M, Majerski K, Marjanović M, Šumanovac-Ramljak, T. Adamantane deriv-

atives of aza-crown ethers and their use in treatment of tumor. Application number: 381-03/09-010/0355

DONATION

Sonja Levanat and the Laboratory for Hereditary Cancer received a Terry Fox donation for genetic research on inherited predisposition for breast and ovarian cancer.

FORMATION OF NEW SOCIETY

The new society was formed and located at the Ruđer Bošković Institute: Croatian Association of Cancer Research (CACR or HDIR), part of the European Association for Cancer Research. First elected president is Sonja Levanat, EACR Council Member.

PROGRAMS AND PROJECTS

Programs supported by the Ministry of Science, Education and Sports

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

Projects supported by the Ministry of Science, Education and Sports

1. Molecular characteristics of the myo-fibroblasts in the Dupuytren's disease, Krešimir Pavelić
2. Role of membrane peptidases on tumour and normal cells, Jelka Gabrilovac
3. Epigenetic and Immunomodulatory Changes in Malignant Head and Neck Tumors, Koraljka Gall Trošelj
4. Aberrant DNA methylation in HPV associated lesions, Magdalena Grce
5. Obtaining the structures like Langerhans islets from mouse stem cells, Mirko Hadžija
6. The role of nm23 genes in oral squamous cell carcinoma, Maja Herak Bosnar
7. Molecular genetics and pharmacogenetics of gastrointestinal tumours, Sanja Kapitanović
8. The mechanism(s) of cholesterol action in Alzheimer's disease, Silva Katušić Hećimović
9. The role of different cell death responses to DNA-damage treatment, Marijeta Kralj
10. Signal transduction in tumours: Hh-Gli interactions and therapeutic potential, Sonja Levanat
11. Cytochrome P450 monooxigenas and tumor appearance in ageing and oxidative stress, Tatjana Marotti
12. Pharmacogenomics and proteomics of serotonergic and catecholaminergic system, Dorotea Muck-Šeler
13. Gene therapy of tumours by modulating the molecules of immune system, Jasminka Pavelić
14. Stress, GABA-A receptors and mechanisms of action of neuropsychoactive drugs, Danka Peričić
15. Molecular basis and treatment of psychiatric and stress related disorders, Nela Pivac
16. New approaches in the treatment of malignant diseases, Marko Radačić
17. The role of p53/p73 protein network in soft tissue sarcoma, Neda Slade
18. Molecular characterisation of S-adenosylhomocysteine deficiency in humans, Oliver Vugrek
19. Lipids, free radicals and their second messengers in integrative oncology, Neven Žarković

Research, developmental and international projects

1. Therapeutic effects of mushroom extracts, (HITRA, Mislav Jurin)
2. Lipidomics of Alzheimer's disease (Croatian National Science Foundation, Marko Košiček, predoctoral fellowship).
3. The mechanism(s) of cholesterol action in Alzheimer's disease (Silva Katušić Hećimović, Bilateral project with USA, co-investigator: Alison Goate)

4. Hereditary Breast Cancer predisposition in Croatia and Hungary', (Croatian Hungarian Intergovernmental S&T Cooperation Programme 2008-2000, Sonja Levanat, Croatia, Edith Olah, Hungary)
5. Integrating and Strengthening Genomic Research in South East Europe (INTEGERS) FP7-REGPOT-2007-1 (Fran Borovečki, members of Coordination Committee: Dorotea Muck-Šeler, Nela Pivac)
6. Genetic testing of monogenetic diseases: cystic fibrosis, non-sindromic deafness, Rett syndrome, (Clinical Hospital Split, Children's Hospital Zagreb, Jasminka Pavelić)
7. Genetic factors as markers of suicide (Nela Pivac, Bilateral Cooperation with Slovenia; co-investigator: Dorotea Muck-Šeler)
8. The study of subcellular localization and dynamics of NDPK A and B subunits (Nm23-H1 and Nm23-H2) (Maja Hrak Bosnar billateral colaboration with France, Cogito)
9. The role of p73 in cell cycle control (Bilateral collaboration with France, Cogito, Neda Slade)
10. Molecular dynamics of S-Adenosylhomocysteine hydrolase (SAHH) and its role in regulation of gene expression. (Oliver Vugrek (IRB) and Yaron Shav-Tal (Bar-Ilan University, Israel).
11. COST (European Cooperation in the field of Scientific and Technical Research) Action B35 "Lipid Peroxidation Associated Disorders" in the Domain Biomedicine and Molecular Biosciences, Action Chair Neven Žarković
12. Support of human bone growth in vitro by bioactive glass and 4-hydroxynonenal, (Austrian National Bank Jubileums Fond Research Grant, Renate Wildburger (LKH Graz) and Neven Žarković)
13. Novel, genuine assays for lipid peroxidation analyses in experimental oncology, (Bilateral project on scientific and technological research collaboration with France – COGITO, Neven Žarković)
14. Modifying drug resistance by oxidative stress and antioxidants (Bilateral Hungarian – Croatian Scientific and Technological Collaboration project, Neven Žarković)

SELECTED ORGANIZED CONFERENCES

1. Pivac N, Muck-Šeler D: Fourth Croatian symposium on stress related disorders: stress and health, with international collaboration, Rabac, Croatia, June 4-6, 2009.
2. Pavelić J: Eight Balkan meeting on human genetics, Cavtat-Dubronik, Croatia, May 14-17, 2009.

SELECTED LECTURES

1. Gall Trošelj K Epigenomics and Translational Research: Challenges and Perspectives. TRX09 (Translational Research Excellence Conference 09), Brisbane, Australia, October 23, 2009.
2. Kralj M "Biomedical Potentials of Crown Ethers: Novel Antitumor Compounds on the Rise?" XXI Croatian meeting of chemists and chemical engineers. Trogir, Croatia. April, 19 – 22, 2009.
3. Levanat S Hedgehog-Gli interactions and therapeutic potential in proliferative tumors of the ovary "14th World Congress on Advances in Oncology and 12th International Symposium on Molecular Medicine", Loutraki, Greece, October 15-17,2009.
4. Levanat S Molecular Genetic Events in Skin Cancer: "1st Meeting of Experts for the Quality of Life Problems in the Senior Population, 4th Meeting of Experts for Influence in Optical Radiations & Electromagnetic Fields on Human, 3rd International Congress of Croatian Association for Protection of non Ionizing Radiation 'Albert Einstein'", Opatia, Croatia, October 23.-15, 2009.
5. Muck-Šeler D Serotonergic system in Alzheimer's disease. Sixth psychogeriatric meeting, Terme Laško, Slovenia, April 23-24, 2009.
6. Pavelić J, Rozman K Current molecular diagnostic techniques for the detection of microbial pathogens causing infective diseases. 7. Bedjaničev simpozij – Infektologija nekoč, danes, jutri, Maribor, Slovenija, May 29 - 30, 2009.

7. Pivac N Genetic markers in suicidal and non-suicidal veterans with combat related PTSD. "Wounds of war II: adressing PTSD in peace-keeping and combat troops", Hotel Amerika-Holzer, Klopeiner See, St Kantian, Austria, October 18-21, 2009.
8. Pivac N Gene polymorphism in combat related PTSD. Synapsa Neuroscience Conference '09, Ljubljana, Slovenia, September 26-29, 2009.
9. Pavelić K Forward Look: Toward the preventive (presimptomatic) medicine in the light of high-throughput (-0mics) techniques. European Medical Research Councils (EMRC) 55th Plenary Meeting of the Standing Committee. Copenhagen, Denmark, October 13-14, 2009.
10. Pavelić K Croatian position on developing scientific strategy: from the perspective of small country. UNESCO General Conference 35th session. Major Program II – Natural Sciences. Paris, October 15-16, 2009.
11. Slade N, Brdar B, Zorić A, Tomić K, Jakovina T, Medverec Z, Dittrich D, Nikolić J, Moriya M, Wu L, Grollman AP, Jelaković B (2009) p53 mutations as fingerprints for aristolochic acid - an environmental carcinogen in endemic (Balkan) nephropathy. Recent Advances in Balkan Endemic Nephropathy Research, Belgrade, Serbia, April, 17-18, 2009.

SELECTED PUBLICATIONS

Selected research articles

1. Bago R, Pavelić J, Maravić Vlahoviček G, Herak Bosnar M: Nm23-H1 promotes adhesion of CAL 27 cells in vitro. *Mol Carcinogenesis* **48** (2009), 779.
2. Ćaleta I, Kralj M, Marjanović M, Bertoša B, Tomić S, Pavlović G, Pavelić K, Karminski-Zamola, G: Novel Cyano- and Amidino- Benzothiazole Derivatives: Synthesis, Antitumor Evaluation, X-ray and QSAR Analysis. *J Med Chem* **52** (2009), 1744.
3. Ester K, Hranjec M, Piantanida I., Ćaleta I, Jarak I, Pavelić K, Kralj M, Arminski-Zamola G: Novel derivatives of pyridylbenzol/b/thiophene-2-carboxamides and benzo/b/thienol/2,3-c/napthyridin-2-ones: Minor structural variations provoke majoer differences of antitumor action mechanisms. *J Med Chem* **52** (2009), 2482.
4. Kraljević Pavelić S, Sedić M, Hock K, Vučinić S, Jurišić D, Gehring P, Scott M, Shlapbach R, Čačev T, Kapitanović S, Pavelić K: An integrated proteomics approach for studying the molecular pathogenesis of Dupuytren's disease. *J Pathol* **17** (2009), 524.
5. Nicula FA, Anttila A, Neamtiu L, Zakelj MP, Tachezy R, Chil A, Grce M, Kesić V: Challenges in starting organised screening programmes for cervical cancer in the new member states of the European Union. *Eur J Cancer* **45** (2009), 2679.
6. Poljak-Blazi M, Morana Jaganjac M, Mustapic M, Pivac N, Muck-Seler D: Acute immunomodulatory effects of iron polyisomaltosate in rats. *Immunobiology* **214** (2009), 121.
7. Radulescu R T, Poznić M, Pavelić K: Complex formation between metabolic enzymes in tumor cells: unfolding the MDR1-IDE paradigm. Letter to the Editor. *Mol Cancer Ther* **8** (2009), 3171.
8. Sredoja Tisma V, Basta-Juzbasic A, Jaganjac M, Brcic L, Dobric I, Lipozencic J, Tatzber F, Zarkovic N, Poljak-Blazi M: Oxidative stress and ferritin expression in the skin of rosacea patients. *J Am Acad Dermatol* **60** (2009), 270.
9. Šimunović M, Perković I, Zorc B, Ester K, Kralj M, Hadjipavlou-Litina D, Pontiki E: Urea and carbamate derivatives of primaquine: synthesis, cytostatic and antioxidant activities. *Bioorg Med Chem* **17** (2009), 5605.
10. Vlainić J, Peričić D: Effects of acute and repeated zolpidem treatment on pentylenetetrazole-induced seizure threshold and on locomotor activity: Comparison with diazepam. *Neuropharmacology* **56** (2009), 1124.
11. Vugrek O, Belužić R, Nakić N, Mudd SH: S-Adenosylhomocysteine hydrolase (AHCY) deficiency: Two novel mutations with lethal outcome. *Human Mutation* **30** (2009), E555.

Review articles

1. **Bosnar MH**, Bago R, Cetkovic H. Subcellular localization of Nm23/NDPK A and B isoforms: a reflection of their biological function? Mol Cell Biochem 2009: 329: 63.
2. **Grce M.** Primary and Secondary Prevention of Cervical Cancer. Expert Rev Mol Diagn 2009: 9: 851.
3. **Kapitanović S**. Molecular genetics and pharmacogenetics in pediatric oncology (in Croatian: Molekularna genetika i farmakogenetika u onkologiji dječje dobi) Paediatr Croat 2009; 53: 193.
4. **Slade N**, Moll UM, Brdar B, Zorić A, Jelaković B. p53 mutations as fingerprints for aristolochic acid – an environmental carcinogen in endemic (Balkan) nephropathy. Mutat Res -Fundam. Mol Mech Mutagen 2009: 663: 1.
5. **Šagud M**, Mihaljević-Peleš A, Mück-Šeler D, Pivac N, Vuksan-Čusa B, Brataljenović T, Jakovljević M. Smoking and schizophrenia. Psychiatria Danubina 2009: 21: 371

Chapters in books

1. **Muck-Šeler D**, Šagud M, Pivac N, Mihaljević Peleš A, Jakovljević M: Neurobiology of depresssion. In: Antidepressants in clinical practice - Editors: Mihaljević Peleš A, Sagud M, (in Croatian). Medicinska naklada, Zagreb, 2009, pp 9-17.
2. **Šagud M**, Mihaljević Peleš A, Muck-Šeler D, Pivac N: Mechanism of action of antidepressants. In: Antidepressants in clinical practice - Editors Mihaljević Peleš A, Sagud M, (in Croatian). Medicinska naklada, Zagreb 2009, pp 19-30.

Division of Marine and Environmental Research

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

DIVISIONAL ORGANIZATION

Head: Tarzan Legović

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

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

OVERVIEW OF THE DIVISION

The mission of the Division is to contribute, by way of fundamental and applied research in environmental systems, processes and states, towards an optimum in environmental management for the benefit of our country and the world.

During 2009, division scientists worked on more than 50 research projects contracted with 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. Results were published in over 60 scientific papers in journals indexed by Current Contents, 13 invited lectures were held and one conference was organized. In addition, 4 graduate schools were coordinated, one M.Sc. and 8 Ph.D theses were defended under the mentorship of Division scientists. Finally, 21 undergraduate and 70 post-graduate courses were given at universities in Croatia and abroad.

TOP ACHIEVEMENTS

Iron (III)-complexes engaged in the biochemical processes in seawater

Fe^{3+} complexes with succinic acid, a ligand naturally present in seawater, were investigated and characterized in aqueous

solutions by square-wave and cyclic voltammetry and confirmed by UV-Vis spectra. Conditional stability constant of $[Fe(suc)_2(OH)_2]$ complex was calculated (Cmuk et al., 2009).

Natural and anthropogenic sources of Hg, Cd, Pb, Cu and Zn in seawater and sediment of NP Mljet

In the Malo Jezero lake, fresh karstic spring water generated by flooding, and weathering of dolomites, are the main sources of naturally elevated Cd, Pb and Zn concentrations. In the Veliko Jezero lake, enhanced Cu and Zn contents originate from anthropogenic input (tourism and agriculture). Distributions of the Pb and Zn in the water columns of both lakes are influenced by natural aragonite precipitation and sedimentation. Exceptionally high total Hg concentrations of 24.2 and 33.7 ng/L in the water column of Malo Jezero, suggest an airborne input (Cuculić et al., 2009).

Kinetic and equilibrium studies of copper-dissolved organic matter complexation

The water column of the stratified Krka River estuary was analyzed to better define and describe conditions when in such an oligotrophic environment (dissolved organic carbon content under 1 $mg_C L^{-1}$) an increase in total copper concentration above 12 nmol/L could enhance the free copper concentration to a level considered potentially toxic for microorganisms (10 pmol/L) (Louis et al., 2009a).

Climatic 60-years records from tufa

A 60-year record (1938-1998) of stable isotope compositions of carbon and oxygen, as well as trace metal (Mg, Sr, Ba) concentrations in a laminated tufa precipitated in a short artificial tunnel of HE Jaruga on a non-equilibrium groundwater-fed karstic river have been investigated. Obtained chemical and isotopic records are compared to hydrometeorological data, available for the last 48 years. An attempt is made to relate isotopic and geochemical variations to environmental parameters (Lojen et al., 2009).

Electrochemical characterization of different sulfur species in model solutions and anoxic natural samples

A proposed electrochemical approach was tested and intercalibrated with spectrophotometric measurements during investigation of sulfur species distribution and speciation in different anoxic aquatic environments (Rogoznica Lake, Croatia and Pavin Lake, France). The chosen study sites have an interesting variety of conditions which influence significant changes in trace metal and sulfur speciation as well as their distribution (solubility) between truly dissolved and colloidal phases across redox interfaces. The lakes differ in chemical conditions since Rogoznica Lake is a seawater lake containing high sulphide waters (up to 10^{-2} M) in the bottom layer and Pavin Lake is a freshwater, crater lake enriched with high metal concentrations (Fe, Mn up to 10^{-3} M) (Bura Nakić et al., 2009).

Constant current chronopotentiometric stripping for characterization of sulphated polysaccharides

It is shown that sulphated polysaccharides are catalysts in the evolution of hydrogen on a mercury electrode. Polysaccharides play important roles in cellular recognition and are involved in abnormal social behaviors in cancer cells. In seawater they are most abundant among organic compounds being excreted from phytoplankton and present in the whole water column, mostly as complex heteropolysaccharides. This paper opens the door for electrochemical analysis of a class of biomacromolecules (Strmečki et al., 2009).

Multivariate statistical analysis of the distribution patterns of carbohydrates and surface-active substances in the northern Adriatic Sea

Dissolved and particulate carbohydrates (DTCHO and PTCHO) and surface-active substances concentrations and relative acidities (SAS_T and Ac_r) were studied in the northern Adriatic Sea on data collected from 1998 to 2005. This work provides the first rigorous statistical analysis performed on a large data set, allowing quantitative assessment of the observed differences. It was shown that mucilage years in the northern Adriatic were characterized by different patterns of the four organic matter parameters (Tepić et al., 2009).

Copper complexing ligands and organic matter characterization in the northern Adriatic Sea

The study of dissolved organic ligands capable of complexing copper ions (L_T) was conducted in the Northern Adriatic Sea in the period from 2006-2008. The majority of organic ligands responsible for Cu binding in surface water originate from new phytoplankton production promoted by river borne nutrients. Older, transformed organic matter, possessing higher relative acidity, is the main contributor to the pool of organic ligands that bind copper in the bottom samples. It was estimated that ~9 % of DOC in surface samples and ~12 % of DOC in the bottom samples are present as ligands capable of complexing copper ions (Plavšić et al., 2009).

Characterization and seasonal variations of surface active substances in the surface microlayers of the coastal middle Adriatic Sea

Surface micro-layer (ML) samples were collected in different seasons over a long time period in the coastal area of the middle Adriatic Sea including the seawater Rogoznica lake and the semi-enclosed estuarine Martinska station. Natural surface microlayers were studied as original samples and as ex-situ reconstructed films after previous extraction by organic solvents of different polarities. Seasonal variability of both SAS concentrations and of inhibitory effects was observed at both locations. The comparison of adsorption characteristics for model lipids of different polarities and those of transferred ex-situ reconstructed films has revealed that different types of lipid material were present in each ex-situ film of the same micro-layer (Frka et al., 2009).

On the mechanism of crystallization of silicalite-1 in heterogeneneous systems (Hydrogels)

The design of zeolites with pre-defined features requires the understanding of their nucleation and growth mechanisms. Because of the wide applications of zeolites as catalysts, molecular sieves, additives etc, there is a growing need to purpose-tailor and control the desired performance of zeolites. Although there are well established techniques to measure the bulk structure of zeolites, the external surface structure is studied insufficiently, except some studies performed by HR-TEM. In this study atomic force microscopy (AFM) was used to investigate the very early stages of nucleation and crystallization on the surface of a gel precursor (Kosanović et al., 2009).

Improvement of electrochemical impedance technique used for electrode characterization.

It is shown that impedance analysis of higly-capacitive and very low impedance electrodes, such as thin film polyaniline modified electrodes, should be performed using a carefully designed three-electrode cell and

analysis procedure involving impedance related to all elements of the cell (Horvat-Radošević and Kvastek, 2009).

Metal accumulation in fish hepatic cytosol

Indigenous specimens of European chub from the Sava River (Croatia) were used as bioindicator organisms for the assessment of metal accumulation. Liver was selected as the target organ and metal concentrations (Zn, Cu, Fe, Mn, and Cd) were determined in two fractions of hepatic cytosol. Concentrations of Zn and Fe were significantly higher in the untreated compared to heat-treated cytosol. On the contrary, Cu, Mn and Cd were predominantly present in the heat-treated cytosol, which contains metallothioneins. In both fractions of hepatic cytosol, the nonessential metal Cd showed a statistically significant increase from the upstream sites toward the downstream site Jasenovac. Hence, Cd concentrations in the hepatic cytosol of European chub has been recommended as an early-warning marker of fish chronic exposure (Podrug et al., 2009).

Figure 1. Pomphorhynchus laevis.

Natural causes of metallothionein variability in fish gills

The possible causes of the variability of gill metallothionein (MT) levels were studied on 182 specimens of 2- and 3-year old European chub (Squalius cephalus L.) from the Sava River, Croatia. The most pronounced differences in MT levels were obtained between two periods of different metabolic activities, April/May 2006 vs. September 2005 and 2006. The site-specific MT variability indicates, that due to low dissolved metal concentrations in the Sava River water, MT levels are more affected by biotic factors such as gill mass than by metal exposure. Therefore, gill MT levels reported in this study are considered the constitutive levels characteristic for young chub specimens (Dragun et al., 2009).

NEW EQUIPMENT

Modular high performance liquid chromatography (Figure 2 HPLC), PerkinElmer HPLC Series 200, with DAD detector Series 200 EP (UV/VIS range 190-700 nm), autosampler Series 225 with Peltier tray, quaternary pump, 5-channel vacuum degassing system, Peltier column oven, Gilson fraction collector and software packages TotalChrom Workstation and IRIS TurboScan200. Instrumental set-up equipped with ion-exclusion column is used for the efficient and reproducible separation of water soluble proteins from the tissue cytosol of indigenous fish and shellfish specimens, collected at marine and freshwater sampling sites differently affected by metal pollution (B. Raspor).

Figure 2. HPLC PerkinElmer HPLC instrument Series 200 in the Laboratory for Biological Effects of Metals.

EDUCATION

Division members participated in the coordination of four graduate school programmes. These include: Biophysics with the University of Split, Environmental Management and Oceanography with the University of Zagreb, and Environmental Protection and Nature Conservation with the University J.J. Strossmayer in Osijek.

AWARDS

Award to Martina Rožmarić Mačefat: The Croatian Radiation and Protection Association award for best scientific publication by a young scientist in 2008-2009. Martina Rožmarić Mačefat received this award for her research of new methods for determination of low level activities of alpha and beta emitters in natural samples. Developed methods are accredited by Croatian Accreditation Agency according to HRN EN ISO/IEC *17025*:2007 and used in daily laboratory work (Rožmarić et al., 2009).

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sports

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

Program supported by the Ministry of Science, Education and Sports

1. Biogeochemical processes and environmental risk, Marijan Ahel

Selected Research, developmental and international projects

1. Direct determination of arsenic species in natural ecosystems by electrochemistry and modeling of its speciation, D. Omanović (ECO-NET, French-Croatian-Bosnian cooperation).
2. Integration of geo-chemical laboratory techniques, in situ field measurement, and hyperspectral air-borne remote sensing for environmental risk assessment, S. Frančišković-Bilinski (Hungarian-Croatian bilateral cooperation).
3. Reference Laboratory, B. Ćosović, D. Hršak, Z. Kozarac and B. Raspor (Ministry of Regional Development, Forestry and Water Management, Water Management Directorate).
4. Marine science and coastal management in the Adriatic Western Balkan, An educa-

tion and research network, B. Ćosović and P. Wassmann (Norwegian cooperation programme on research and higher education).

5. A complex study of marine organic matter characterization in seas of the European coastal zone, B. Gašparović and G. Kattner (Bilateral collaboration with Alfred Wegener Inst Polar & Marine Res, Bremerhaven, Germany).
6. 6. On line toxicity sensors based on modification of membrane organisation, B. Gašparović and L.A. Nelson (NATO science for peace and security programme).
7. Complex investigation of organic aerosols in rural, urban and marine environment, Z. Kozarac, and G. Kiss (Bilateral collaboration with Air Chemistry Group of the Hungarian Academy of Sciences at University of Pannonia, Veszprém).
8. Biogeochemical processes in anoxic environments: electrochemistry as an alternative tool for trace metals and sulfur determination, I. Ciglenečki-Jušić and G. Inzelt (bilateral collaboration with "Lorand Eötvös" University in Budapest, Department for physical chemistry, Hungary).
9. Study of biogeochemical sulfur cycling in water column of Rogoznica Lake (Croatia) by combination of chromatographic and electrochemical techniques, I. Ciglenečki-Jušić and T. Ferdelman (Bilateral collaboration with Max-Planck-Institute for Marine Microbiology, Bremen, Germany).
10. Biogeochemical processes in anoxic environment: Characterization of metal sulfide nanoparticles by electrochemical methods, I. Ciglenečki-Jušić and E. Viollier (Bilateral collaboration with University of Paris, IPGP, France).
11. Biogeochemistry of sulfur, carbon, nutrients and redox sensitive elements in hypoxic/ anoxic aquatic environments, I. Ciglenečki-Jušić and Minhan Dai (Bilateral collaboration with State Key Laboratory of Marine Environmental Science, Xiamen University, China).
12. Monitoring of freshwater fishery: fishing area of the Rivers Sava and Sutla, E. Teskeredžić (Ministry of Agriculture, Fishery and Rural Development).
13. AFM study of the crystallization of synthesized zeolites, V. Svetličić and T. Mišić (Bilateral Cooperation project with Eötvös Loránd University, Budapest, Hungary).

SELECTED INVITED LECTURES

1. Cuculić V, Cukrov N, Kwokal Ž, Jalžić B. Distribution of Hg, Cd, Pb, Cu and Zn in water columns and sediments of two anchialine caves in Mljet National Park – Croatia, Anchialine ecosystems: Reflection and prospects, Palma de Mallorca, Spain, November 17-20, 2009.
2. Legović T, Klanjšček J, Geček S. Maximum sustainable yield and species extinction in ecosystems, ISEM 2009 Conference , Quebec City, October 6-9, 2009.
3. Cukrov N, Jalžić B, Bilandžija H, Cukrov M. Research history and anchialine cave characteristic in Croatia, Anchialine ecosystems: Reflection and prospects,Palma de Mallorca, Spain, November 17-20, 2009.
4. Žic V, Cukrov N, Cuculić V, Kwokal Ž, Jalžić B. Iodine and nutrient speciation in anchialine cave waters (Bjejajka Cave, East Adriatic Coast), Anchialine ecosystems: Reflection and prospects. Palma de Mallorca, Spain, November 17-20, 2009.
5. Ciglenečki I. Rogoznica Lake (Croatia), a unique anoxic seawater system on the Adriatic coast, Max Planck Institute for Marine Microbiology, Bremen, Germany, November 2009.
6. Bura-Nakić E, Viollier E, Jézéquel D, Thiam A, Ciglenečki I. Reduced sulfur and iron species in anoxic water column of Lake Pavin, International Meeting Lake Pavin and Other Meromictic Lakes, Clermont Ferrad University, France, May 2009.
7. Frka S, Gašparović B. Particulate lipids in the atlantic surface ocean (ANT XXV-1 cruise). Symposium & workshop: The expedition ANT-XXV/1 of the research vessel „Polarstern" Bremerhaven - Cape Town in 11/2008: Biogeochemical fluxes and short-term molecular changes in the Atlantic surface ocean. Bremerhaven, October 12-14, 2009.

8. Gašparović B, Frka S, Kozarac Z, Koch B, Kattner G. Methods for the physico-chemical qualitative and quantitative characterization of sea-surface microlayer surfactants. COST 735 Meeting on The role of surfactants in air-sea gas transfer. Plymouth, UK, March 18-21, 2009.
9. Svetličić V, Mišić T, Žutić V, Urbani R, Boulgaropoulos B. Supramolecular organization and process of marine gel network formation visualized by atomic force microscopy, Regional Biophysical Conference, Linz, Austria, February 10-14, 2009.

SELECTED ORGANIZED CONFERENCES

1. Regional Biophysical Conference 2009, 10-14 February, Linz, Austria (Svetličić V, International Advisory Board).

SELECTED PUBLICATIONS

1. Cmuk P, Piantanida I, Mlakar M: Iron (III)-complexes engaged in the biochemical processes in seawater. I. Voltammetry of Fe(III)-succinate complexes in model aqueous solution. *Electroanalysis* **21** (2009), 2527.
2. Cuculić V, Cukrov N, Kwokal Ž, Mlakar M: Natural and anthropogenic sources of Hg, Cd, Pb, Cu and Zn in seawater and sediment of Mljet National Park, Croatia. *Estuarine, Coastal and Shelf Science* **81** (2009), 311.
3. Lojen S, Trkov A, Ščančar J, Vázquez-Navarro JA, Cukrov N: Continuous 60-year stable isotopic and alkali element records in a modern laminated tufa (Jaruga hydroelectric power plant, river Krka, Croatia). *Chemical Geology* **258** (2009), 242.
4. Louis Y, Garnier C, Lenoble V, Mounier S, Cukrov N, Omanović D, Pižeta I: Kinetic and equilibrium studies of copper-dissolved organic matter complexation in water column of the stratified Krka River estuary (Croatia). *Marine chemistry* **114** (2009), 110.
5. Bura-Nakić E, Helz GR, Ćosović B, Ciglenečki I: Reduced sulfur species in a stratified sea-water lake (Rogoznica Lake, Croatia); seasonal variations and evidence for organic carriers of reactive sulfur. *Geochim Cosmochim Acta* **73 (**2009), 3738.
6. Strmečki S, Plavšić M, Ćosović B, Ostatna V, Paleček E: Constant current chronopotentiometric stripping of sulphated polysaccharides. *Electrochemistry Communications* **11** (2009), 2032.
7. Plavšić M, Gašparović B, Strmečki S, Vojvodić V, Tepić N: Copper complexing ligands and organic matter characterization in the northern Adriatic Sea. *Estuarine, Coastal and Shelf Science* **85** (2009), 299.
8. Tepić N, Gašparović B, Ahel M: Multivariate statistical analysis of the distribution patterns of carbohydrates and surface-active substances in the northern Adriatic. *Mar Chem* **114** (2009), 37.
9. Frka S, Kozarac Z, Ćosović B: Characterization and seasonal variations of surface active substances in the natural sea surface micro-layers of the coastal Middle Adriatic stations. *Estuarine Coastal and Shelf Science* **81** (2009), 555.
10. Sondi I, Bišćan J, Vdović N, Srečo DŠ: The electrokinetic properties of carbonates in aqueous media revisited. Colloids and Surfaces A. *Physicochemical and Engineering Aspects* **342** (2009), 84.
11. Kosanović C, Havancsák K, Subotić B, Svetličić V, Mišić T, Cziráki A, Huhn G: A contribution to understanding the mechanism of crystallization of silicalite-1 in heterogeneneous systems (Hydrogels). *Micropor Mesopor Mat* **123** (2009), 150.
12. Horvat-Radošević V and Kvastek K: Three-electrode cell set-up electrical equivalent circuit applied to impedance analysis of thin polyaniline film modified electrodes. *J Electroanal Chem* **631** (2009), 10.
13. Dutour-Sikirić M, Janeković I, Kuzmić, M: A new approach to bathymetry smoothing in sigma-coordinate ocean models. *Ocean Modelling* **29** (2009), 128.
14. Rožmarić M, Gojmerac Ivšić A, Grahek Ž: Determination of uranium and thorium in complex samples using chromatographic separation, ICP-MS and spectrophotometric detection. *Talanta* **80** (2009), 352.

15. Dragun Z, Podrug M, Raspor B: The assessment of natural causes of metallothionein variability in the gills of European chub (Squalius cephalus L.). *Comparative Biochemistry and Physiology Part C* **150** (2009), 209.
16. Podrug M, Raspor B, Erk M, Dragun Z: Protein and metal concentrations in two fractions of hepatic cytosol of the European chub (Squalius cephalus L.). *Chemosphere* **75** (2009), 843.

CHAPTERS IN BOOKS

1. Čelebić A., Svetličić V., Malina J., Klaić B. Co-Cr-Mo Alloy Surface Features and Composition prior and after Mechanical Polishing and Corrosion in Fluids Simulating Oral Conditions. In: Biomaterials Developments and Applications – Editors: Bourg H, Lisle A, (in English), Nova Science Publishers, Inc., Huntington, New York, 2009.

Center for Marine Research

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

DIVISIONAL ORGANISATION

Head: Nenad Smodlaka

The Centre for Marine Research consists of the following laboratories:

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

OVERVIEW OF THE DIVISION

The mission of the Center for Marine Research is to conduct multidisciplinary studies of processes in the marine environment from sub cellular 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 of the Adriatic Sea for government agencies and in the context of several international projects (INTERREG) regarding protection of the marine environment.

TOP ACHIEVEMENTS

Extreme oceanographic conditions in the northern Adriatic during 2009

Oceanographic parameters (salinity, temperature, dissolved oxygen, transparency, nutrients, chlorophyll *a*, and others) and phytoplankton counts were measured in the northern Adriatic in 2009 within the framework of projects “Jadran”, WICOS and “Strengthening of coastal water monitoring network” during cruises of the Center’s RV “Vila Velbita”.

Collected data, when compared with historical data sets (1972-2008), show that extreme conditions were established in the surface layer during the late winter-spring period, and late autumn.

After a five year period (2003-2007) when the Po River discharge rate had been very low, often with values below the historical minimum, in 2008, and even more intensely in 2009, considerable freshets occurred in spring and autumn. Flow rates significantly higher than two standard deviations from the long-term mean (1917-2008) were measured in February, April-May, and December 2009. Consequently, in those periods,

surface salinity values were near the historical minimum and an extremely high nutrient accumulation was observed.

Extreme and unusual phytoplankton blooms in the northern Adriatic during 2009

Unusually intense blooms of *Skeletonema marinoi* lasted from January till April, while in late autumn remarkably high numbers of the silicoflagellate *Mesocena* sp., and extremely rare heteroflagelate *Hermesinum adriaticum* (Figure 1) were observed. A denser than usual population of dinoflagellates also occurred in summer (Figure 2).

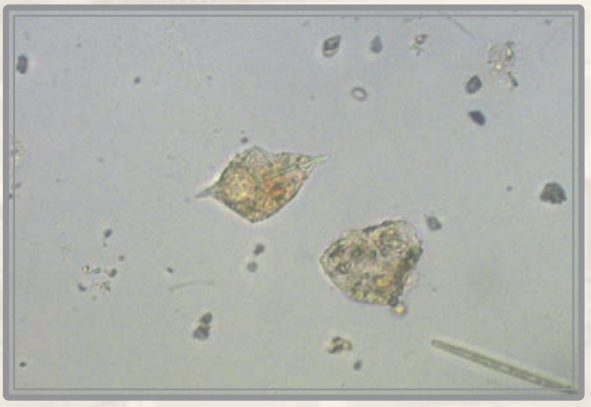


Figure 1. The heteroflagelate Hermesinum adriaticum, an extremely rare species in the northern Adriatic. Light micrograph taken on a Zeiss Axiovert M 200 inverted microscope using phase contrast.

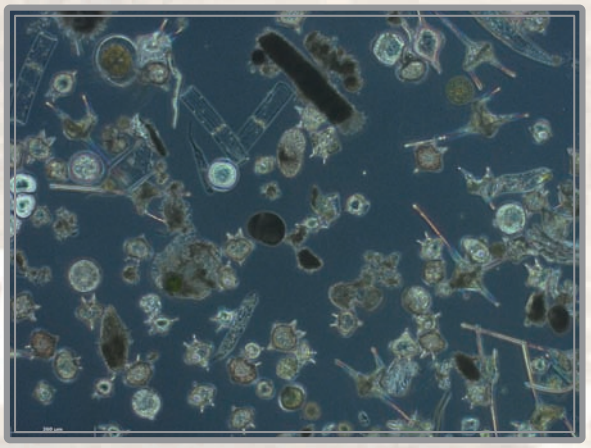


Figure 2. Live net sample of a phytoplankton community dominated by dinoflagellates. Light micrograph taken on a Zeiss Axiovert M 200 inverted microscope using phase contrast.

The observed changes can in part be related to global warming and its consequent extreme climatic fluctuations.

Phytoplankton research improvements

An intercalibration project between the CMR, and the Oceanographic Structure Daphne, Cesenatico, Italy, now allows the combined analysis and quality control of phytoplankton monitoring results established in both institutions for the northern Adriatic. The intercalibration included sampling and sample preparation/fixation as well as species determination, quantification, and biovolume analysis (Figure 3).

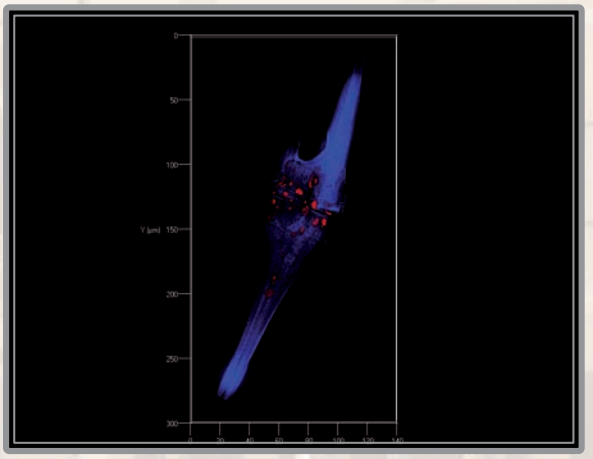


Figure 3. Threedimensional reconstruction of a dinoflagelate cell Ceratium furca after computational optical sectioning on a new fluorescent microscope Zeiss axio imager.

New areas of phytoplankton research and new instruments

New Hardware and Software for computational biology is now used in molecular taxonomy, phylogeny and systematics. A new PCR machine allowed the amplification of more difficult marker sequences as well as an increased throughput. These new analytic capabilities were applied to determine cryptic and toxic species. A new culture chamber allowed the establishment of the CMR culture collection which now holds more than 150

different clonal cultures of northern Adriatic phytoplankton species. Educational efforts in this area included a workshop on advanced light microscopy (RESOLUTION) and a workshop on molecular taxonomy, phylogeny and systematics in phytoplankton research.

Sponge ecology and physiology

A number of investigations in cooperation with the University of Stuttgart demonstrated that the sponge *Aplysina aerophoba* is not a filter feeder *sensu strictu*. Microscopical examinations showed that the sponge is also not feeding on Eucaryotic plankton. This leaves only dissolved organic matter as a possible food source. Therefore the textbook view of sponges being naturally filter feeding organisms has to be revised (Pfannkuchen et al., 2009).

Figure 4. The aspect of a coralligenous community with Aplysina cavernicola sponge.

Characterization and differentiation of oligotrophic waters by culturable particle-attached and free-living bacterial community

A tool based on cellular fatty acids of culturable heterotrophic bacterioplankton was developed in order to characterize and differentiate northern Adriatic, particularly oligotrophic high-salinity, waters. Variances in growing abilities and population dominance of particle-attached and free-living bacteria cultured in three media, Marine Broth, diluted Marine Broth (1:10), and R2 broth were used. Low productive, oligotrophic water layers were characterized by weak culturability, different population dominance of the free-living community in respect to attached counterpart or even growth arrest in response to all media. In both fractions, tested separately, a significant influence of trophic state was present ($p < 0.05$), while the effect of media on fatty acid response was insignificant ($p > 0.05$). The free-living fraction of bacterioplankton is a more informative attribute and can be used solely as an indicator of the water layer trophic condition (Blažina et al., 2009).

Phytoplankton and bacteria alkaline phosphatase activity in the northern Adriatic Sea

The importance of bacterial, phytoplankton and dissolved alkaline phosphatase activity (APA) in the northern Adriatic was investigated. During late spring and summer both communities exploited dissolved organic phosphorus although, taking into account biomass, phytoplankton activity usually dominated over bacterial activity. In autumn an extra P supply from deeper waters drastically reduced phytoplankton APA, though not bacterial APA, in upper waters. In these months bacteria that were degrading phytoplankton produced organic matter were P limited. In deeper waters APA was low and mainly due to the activity of free enzymes (Ivančić et al., 2009).

The distinction of *Aplysina cavernicola* and *A. aerophoba* (Demospongiae) using different biochemical composition of metabolites

Two species of the genus Aplysina (*A. cavernicola* Schmidt, 1862, and *A. aerophoba* Schmidt, 1862) co-occur in the Mediterranean. Since both species display a high degree of phenotypic variability, distinctions based solely on morphological attributes is

not suitable in all cases. For the first time we report an investigation of both Aplysina species along one transect on an underwater slope in the Adriatic, and the successful species distinction using solely the different biochemical composition of metabolites (Kloppel et al., 2009).

Assessment of the ecological status of north-eastern Adriatic coastal waters using macroalgal assemblages

Based on the inclusion of macroalgae in the European Union Water Framework Directive as quality elements for the evaluation of the ecological status of coastal waters, the suitability of one (Ecological Evaluation Index, EEI) of several previously proposed evaluation methods in the particular ecological conditions of the northern Adriatic Sea was tested. When assessed at 1 m depth the spatial scale weighted EEI for the west Istrian coast was 8.1, corresponding to an ecological status class (ESC) value of high. However, data for 3 m depth gave a spatial EEI of 6.72 which corresponds to an ESC value of good. It is concluded that the EEI method may be suitable for the classification of coastal waters in the northern Adriatic only in certain cases (Figure 5) (Iveša et al., 2009).

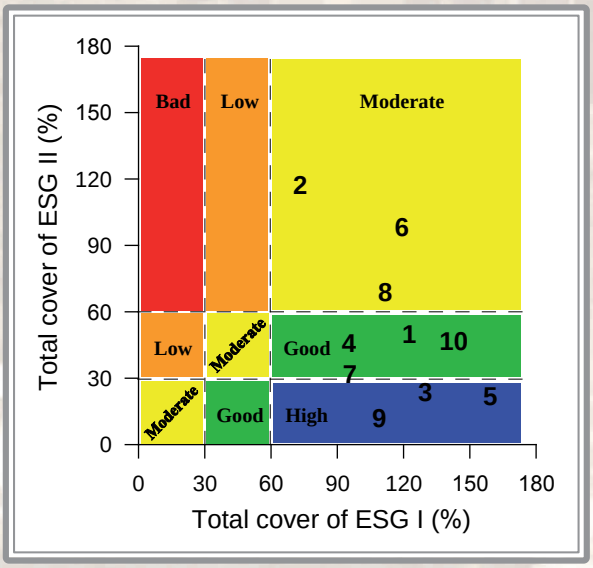


Figure 5. Categorized scatterplots of the macroalgal total cover (%) of ecological status groups (ESG I and ESG II) for locations along the western Istrian coast at 1 m depth.

Biominerals in marine organisms as a tool for monitoring of environmental changes

Studies of biomineral encrustation on a 2,000-year-old bronze sculpture of the famed ancient Greek athlete Apoxyomenos have shown how marine organisms may provide passivating layers for the protection of metal objects and may provide new understanding of how to prevent metal corrosion or develop safer ways to permanently store nuclear waste (Lyons et al., 2009; Medaković, 2009).

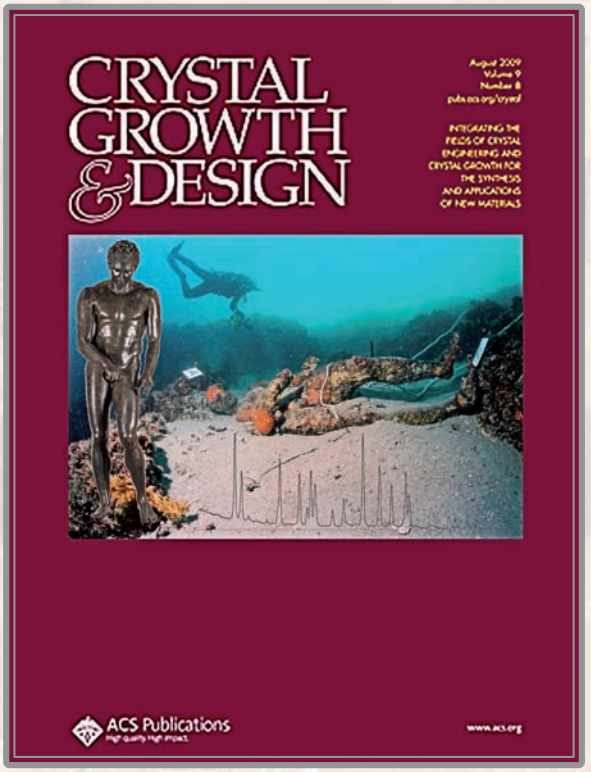


Figure 6. Cover page of the American Chemical Society journal Crystal Growth & Design, August 2009.

Starting biominerals in marine organisms

Research on the appearance of the first biominerals in embryos of marine organisms, using the most modern materials instrumen-

tation including X-ray diffraction, scanning electron microscopy with energy dispersive X-ray analysis and high resolution transmission electron microscopy with selected area electron diffraction, has revealed a method to induce precipitation of the first nucleated crystalline phase in embryos by electron beams (Figure 7).

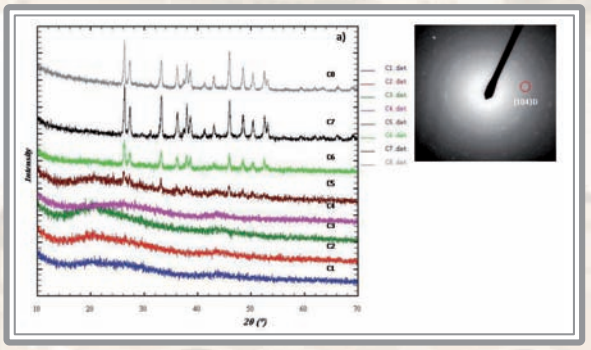


Figure 7. a) X-ray diffractograms of Aplysia punctata embryos, from C1 = 3 days to C8 = 24 days after fertilization. The first aragonite minerals are recorded in the 15 day old embryos of sample C5 b) Corresponding SAED diffraction pattern of the appearance of a crystalline dolomite phase (crystallite size ~10 nm) within the amorphous region in sample C4 (12 day old embryos).

Radioecology

In association with the International Atomic Energy Agency, artificial radioactivity in the northern Adriatic Sea was assessed through ^{137}Cs content in seawater, sediment and marine organisms in different part of marine ecosystem, with results showing that the radio-ecological status of ^{137}Cs in the Adriatic Sea has returned to the pre-Chernobyl accident long-term average level (Figure 8a i 8b).

Fast Micromethod®

The Fast Micromethod® is used not only for human DNA alteration measurements, but also for genotoxicity assessment and estimation of harmful effects of pollution on marine invertebrates. A comprehensive description of this method, its use, detailed descriptions and insights into sample and reagent preparation, fluorescence analyses

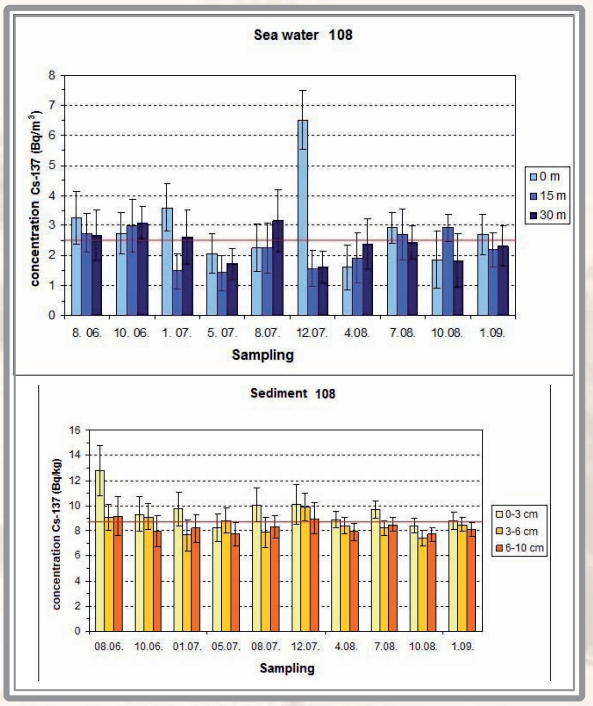


Figure 8. Concentrations of ^{137}Cs in seawater collected at 3 depths (0, 15 and 30 m) and in the sediment layer (0-10 cm) at Station 108 from 2006 to 2009.

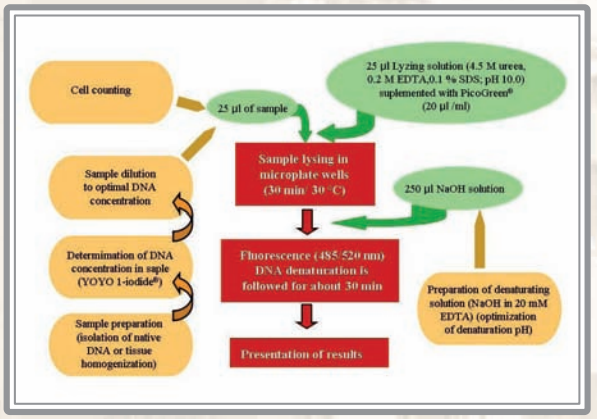


Figure 9. Schematic representation of DNA integrity determination by Fast Micromethod®

and calculation of DNA integrity is critically addressed (Figure 9; Jakšić, 2008).

p53 family research

High sequence conservation of the p53 tumor suppressor gene family members and numerous alternative products expressed

from these genes caused quite a confusion in the nomenclature of non-vertebrate homologs. Our comparative study of genomic structures (Figure 10) and phylogeny of the p53 tumor suppressor gene family has shown strong indications that p63 is the ancestral and the only gene of the p53 family present in Molluscan, as well as other non-vertebrate animals (Štifanić et al., 2009).

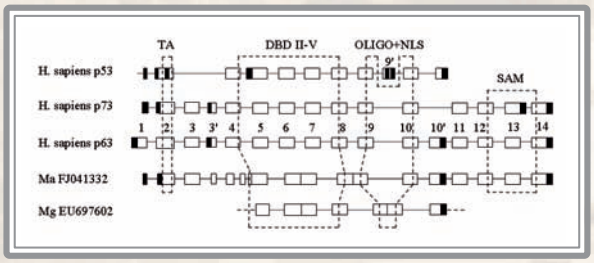


Figure 10. When compared to Vertebrate (human) p53 family gene structures Mya arenaria and Mytilus galloprovincialis homologs resemble the highest similarity to vertebrate p63. For details see Figure 6 in Štifanić et al., 2009.

NEW EQUIPMENT

- Epifluorescence microscope "Zeiss-Imager Z1"
- Growth chamber Memmert ICP700
- Centrifuge „Eppendorf 5415R"
- pH Meter „Radiometer analytical"
- Stereozoom microscope Olympus SZX2-ZB16 with light source
- Benchtop Centrifuge with swing out rotor (Universal 320), Hettich
- Multiparameter Meter HQ40D Hach Lange for water quality monitoring (pH, DO, t, salinity)
- Portable ORP meter Mettler Toledo

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. Under- and post-graduate courses were given at the Universities in Zagreb, Split, Dubrovnik and Osijek.

PROJECTS AND PROGRAMS

Projects supported by the Ministry of Science, Education and Sport

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

Programs supported by the Ministry of Science, Education and Sport

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

Research, developmental and international projects

1. Understanding and manipulating enzymatic and proteomic processes in biomineralization - towards new biomimetic strategies, the creation of tailored nano-scale architectures and environmental monitoring, Davorin Medaković, EU COST Action TD0903 (2009-2013)
2. Proteomique des Molluscques et Biominéralisation (ProMoBio), Davorin Medaković, ECO-NET, Paris France (2008-2010)
3. Development of a nanotechnology-based sensor for marine biotoxins, Daniel Mark Lyons, Zaklada Adris, Republic of Croatia (2009-2012)

4. Design of a new 'immunoassay' for marine biotoxins, Daniel Mark Lyons, Royal Society of Chemistry, United Kingdom (2008-2009)
5. Implementation of the water quality monitoring in the western Istrian coastal sea (northern Adriatic) (WICOS), Tamara Đakovac and Danilo Degobbis, INTERREG IIIA-CARDS/ PHARE, 2006-0017-972009 (2008-2009)
6. Carboanhydrase-Gehalt/Aktivität und Biomineralisation in Mittelmeermuscheln und Schwämmen, Hans C. Schröder, Bojan Hamer, Internationales Büro des Bundesministerium fur Bildung un Forschung (BMBF) (MOE 08/R55, 2008-2009)
7. Coastal cities water pollution control project. Part C1: Strengthening of coastal water monitoring network, Robert Precali, Ministry of the Environmental Protection, Physical Planning and Construction, IBRD 7226/HR (2008-2009)
8. Mapping of marine habitats based on benthic communities, according National Classification of Habitats (NCH) and Natura 2000 Classification. Republic of Croatia Ministry of Culture, State Institute for Nature Protection, Ana Travizi

SELECTED INVITED LECTURES

1. Lyons DM, Medaković D, Marin F (2009) Understanding and manipulating enzymatic and proteomic processes in biomineralization: towards new biomimetic strategies, the creation of tailored nano-scale architectures and environmental monitoring «COST TDP Presentations» (Brussels, Belgium, 12 March 2009).
2. Lyons DM (2009) The coming paradigm shift in biomimetics: proteomics-based control, Faculty of Science, Free University of Brussels (Brussels, Belgium, 13 March 2009).
3. Medaković D (2009) Biomineralization processes in Marine organisms. Laboratoire de Biologie Marine, Université Libre de Bruxelles, Campus du Solbosch (Brussels, Belgium, 13 March 2009).
4. Supić N (2009) Winter oceanographic conditions in the northern Adriatic, Department of Geophysics, Faculty of Natural Sciences, University of Zagreb (Zagreb, 17 June 2009).
5. Medaković D (2009) "Biomineralization Processes in Marine Organisms". Muséum National d'Histoire Naturelle Département Milieux et Peuplements Aquatiques, Equipe "Evolution des biominéralisations" UMR 7208 (Paris, France, 23 June 2009).
6. Degobbis D, Djakovac T, Precali R (2009) Attività del Centro per la Ricerca del Mare di Rovigno finalizzate alla salvaguardia della qualità delle acque, Convegno finale Progetto SAVE COAST (Rovinj, 14 July 2009).

SELECTED ORGANIZED CONFERENCES

School of Conservation Biology of the Croatian Biological Society in affiliation with Ruđer Bošković Institute, Center for Marine Research, Rovinj, 15-23 June 2009. Hamer B. (Vice Chair), Smodlaka N. (Financial director).

SELECTED PUBLICATIONS

Additional publications

1. Blažina M, Iveša Lj, Najdek M: *Caulerpa racemosa*: Adaptive varieties studied by fatty acid composition (Northern Adriatic Sea, Vrsar, Croatia). *Eur J Phycology* **44** (2009), 183.
2. Blažina M, Najdek M, Fuks D, Ruso A, Štifanić M, Pavlinić D: Characterization and differentiation of the oligotrophic waters by culturable particle-attached and free-living bacterial community. *Ecol Indicators* **9** (2009), 1265.
3. Ivančić I, Radić T, Lyons DM, Fuks D, Precali R, Kraus R: Alkaline phosphatase activity in relation to nutrient status in the northern Adriatic Sea. *Mar Ecol Progr Series* **378** (2009), 27.
4. Iveša L, Lyons DM, Devescovi M: Assessment of the ecological status of northeastern

Adriatic coastal waters (Istria, Croatia) using macroalgal assemblages for the European Union Water Framework Directive. *Aquat Conserv* **19** (2009), 14.

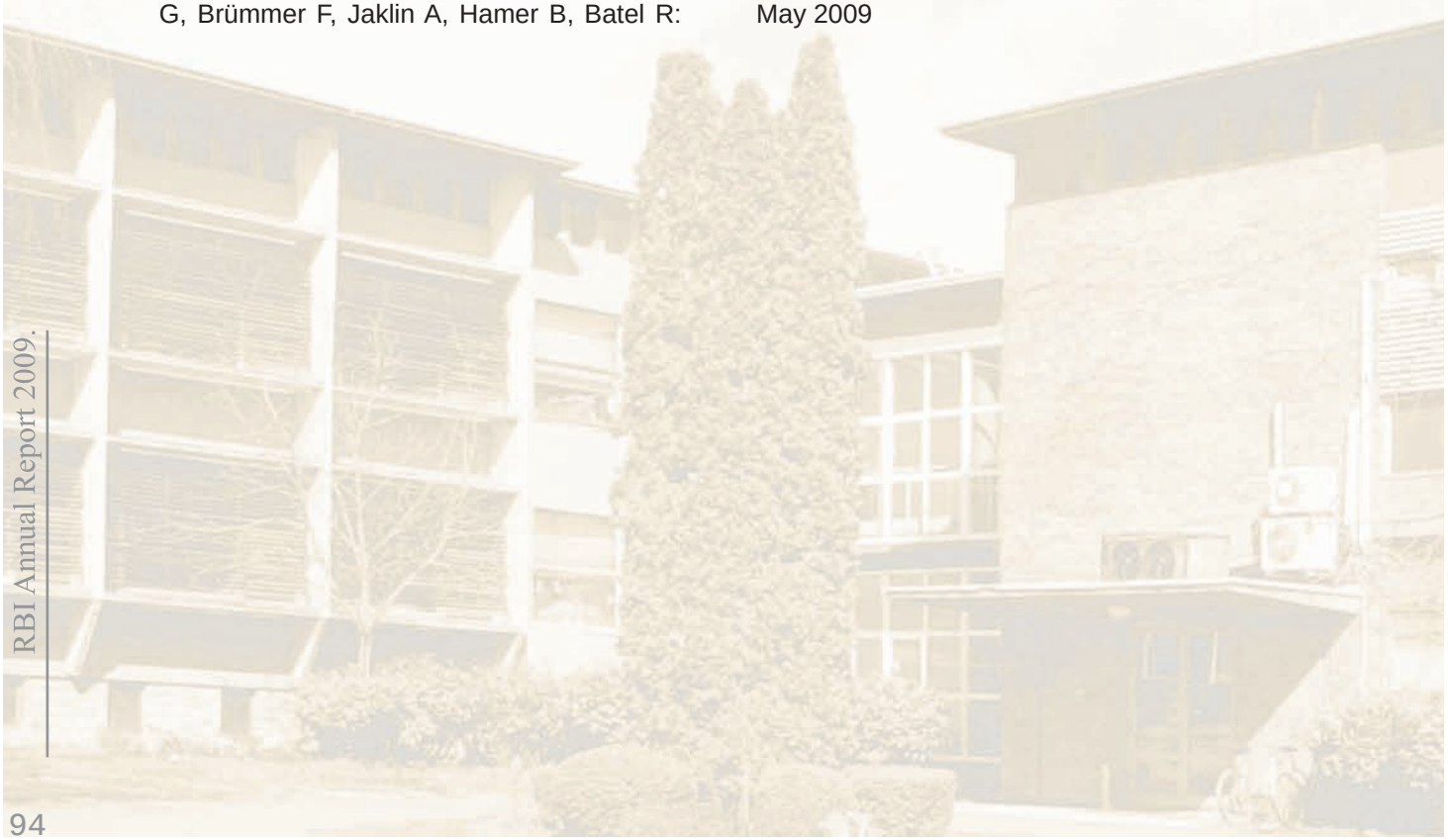
5. Kloppel A, Putz A, Pfannkuchen M, Fritz G, Jaklin A, Proksch P, Brümmer F: Depth profile of Aplysina aerophoba ssp.: morphological, histological and biochemical aspects and their role in species distinction. *Mar Biodiv* **39** (2009), 2-121.
6. Lyons DM, Medaković D, Skoko Ž, Popović S, Rončević S, Pitarević Svedružić L, Karniš I: Biomineralization on an ancient sculpture of the Apoxyomenos; Effects of a metal-rich environment on crystal growth in living organisms. *Cryst Growth Des* **9** (2009), 3671 (*including Cover Art*).
7. Medaković D: 2.000-year-old statue sheds light on seawater corrosion. Information on corrosion control and prevention. *Mater Performance* **48** (2009), 12.
8. Palijan G, Fuks D, Vidaković J: Spatial and temporal distribution of net nitrite and nitrate production on submersed macrophyte *Ceratophyllum demersum* L. *Fresenius Environ Bull* **18** (2009), 64.
9. Pfannkuchen M, Marić D, Godrijan J, Fritz G, Brümmer F, Jaklin A, Hamer B, Batel R: Sponges (Porifera) and eukaryotic, unicellular plankton. A case study on *Aplysina aerophoba*, Nardo 1886 in the northern Adriatic. *J Exp Mar Biol Ecol* **382** (2009), 40-4.
10. Radić T, Šilović T, Šantić D, Fuks D, Mičić M: Preliminary flow cytometric analyses of phototrophic pico- and nanoplankton communities in the northern Adriatic. *Fresenius Environ Bull* **18** (2009), 715.
11. Štifanić M, Mičić M, Ramšak A, Blašković S, Ruso A, Zahn RK, Batel R: p63 in *Mytilus galloprovincialis* and p53 family members in the phylum Mollusca. *Comp Biochem Evol Part B Biochem Evol* **154** (2009), 264.

Chapter in the book

1. **Jakšić Ž.** Assessing the Fast Micromethod as a tool in DNA integrity measurement. In: Progress in DNA Damage Research, Eds. S. Miura and S. Nakano, Nova Publishers, 2008, pp. 349-369

PhD Thesis

Nerlović V, Structure and dynamics of the northern Adriatic soft bottom Bivalvia. Faculty of Science and Mathematics, University of Zagreb, May 2009



Centre for Informatics and Computing

CIR

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

ORGANISATION OF THE CENTRE

Head: Karolj Skala

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

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

centar za informatiku i računarstvo

CIR continues activities related to the national scientific program, projects and international collaboration with highly respected EU FP7 project consortia. The Information systems and Service and maintenance groups are active in the development and maintenance of the RBI's ICT infrastructure, core ICT and other related services in support of scientific personnel.

OVERVIEW OF THE CENTRE

Scientific Research and Development

The mission of the CIR R&D programme is advancement of computer usage in scientific work, based on the development of e-Science technologies as the fourth paradigm of the scientific work platform - knowledge infrastructure to support computation based science.

CIR has experience in signal and image processing, computer graphics, parallel algorithms, 3D visual interfaces and peripherals, including integration of user interfaces and interactive environments in virtual and real space as well as human-machine interaction.

TOP ACHIVEMENTS OR **HIGHLIGHTS IN 2009**

EU projects

- Successful finished the SEE GRID II, EGEE II and CenVis EU FP6 projects.
- Provided three EU FP7 ICT STREP projects funded by European Commission

Development of new technology and equipment and service

- Scientific service development; 3D Protein Data Base Visualisation Generator
- Virtual interaction and design, 3D modelling and 3D printing technologies

Infrastructure support improvements

- Scientific Visualisation Laboratory fully completion and openning.
- Cluster and Grid Infrastructure Room instalation and start to production

eScience Development Activities

During 2009 CIR continued the eScience programme based on ICST (Information Communication Science Technology) on Grid platforms. Inside the framework of the CRO NGI a new cluster was installed at RBI, having 512 processors for furthering scientific research.

The SEE-GRID-SCI (SEE-GRID eInfrastructure for regional eScience) is a project which aims to stimulate widespread eInfrastructure uptake by new user groups extending over the region, fostering collaboration and providing advanced capabilities to more researchers, with an emphasis on strategic groups in seismology, meteorology and environmental protection. In parallel, the project enlarges the regional eInfrastructure to cater to the demands of the communities by increasing the computing and storage resources and involving new partner countries in the region. In the 2009 the SEE-GRID-SCI project has successfully deployed and developed more than 15 applications from three target scientific fields on the Grid infrastructure. The CIR as local coordinator, has developed two applications in the fields of meteorology and environmental protection. The first application is the Weather Research and Forecasting (acronym: WRF-ARW) model used for advanced weather prediction and research purposes using the Grid. The second application is the Regional Ocean Modelling System (acronym: ROMS) which is adopted for the grid execution together with the Division for Marine and Environmental Research at RBI. The steering committee and review meeting was organised by the RBI in Dubrovnik in September 2009. Experts from RBI also participated as trainers and presenters at different training events and conferences in Banja Luka, Instanbul, Zagreb, Dubrovnik, and Opatija.

The EGEE project provides researchers in academia and business with access to a production level Grid infrastructure, independent of their geographic location. The project's main focus is to expand and optimize Europe's largest production Grid infrastructure, namely EGEE, by continuous operation of the infrastructure, support for more user communities, and addition of further computational and data resources and to prepare the migration of the existing production European Grid from a project-based model to a sustainable federated infrastructure based on National Grid Initiatives for multi-disciplinary use. In the EGEE project CIR was working as the part time user support team for the whole EGEE user community across Europe. CIR also participated in dissemination and training activities for local end users. Several training events were organized together with the Faculty of Graphic Arts, University of Zagreb, with the topics: "Rendering Application System", "Photorealistic 3D grid rendering workshop" and others. Much effort was placed on dissemination activities where the scopes and achievements of the EGEE project were presented.

DARIAH (Digital Research Infrastructure for the Arts and Humanities) is an ESFRI roadmap project with the aim to develop and maintain an infrastructure in support of ICT-based research practices across the arts and humanities. In 2009 DARIAH ended the first half of it's preparation phase and achieved many technical and dissemination objectives. Two demonstrators (ARENA, TEI) were built and many small technical experiments on available technologies were carried out. Gathering knowledge on known technologies is very important for creating a plan for the project's construction phase. Col-

laboration was established with other similar projects (CLARIN, CESSDA). In cooperation with CLARIN, DARIAH organized the “Digital Data Storage System - National Strategy Development” round table in Zagreb.

Figure 1. Digital Data Storage System - National Strategy Development round table.

Information Systems development and service usage

The new reservations system engine (http://reservations.irb.hr), which assists both users and employees in charge of shared resources distribution, was developed. It’s core advantages are adaptability and ease of use. The OpenVPN solution has entered the production phase and proven itself to be one of the most requested services. Other projects, commenced and undergoing thorough testing processes, include a web survey system (http://survey.irb.hr), mailing lists administration interface and an LDAP administration front-end. Significant efforts were made to maintain a comprehensive documentation of all activities.

Hardware/network infrastructure

The newly built server, cluster and Grid room, informally referred to as the “red room” (Figure 2), can accommodate up to ten 42Ux600x1000 racks, each one providing 32A of electrical power at bare minimum. It also incorporates state-of-the-art cooling, surveillance and extinguishing systems and a dedicated fiber optics cable uplink.

Figure 2. Cluster and Grid Infrastructure room.

We migrated some of the Institute’s key servers into virtual machines, adopted improved backup procedures and upgraded our webmail solution as well as portable booth-pc running Linux OS. Network security has improved significantly with incorporating new monitoring mechanisms, logging, graphing and of course documenting.

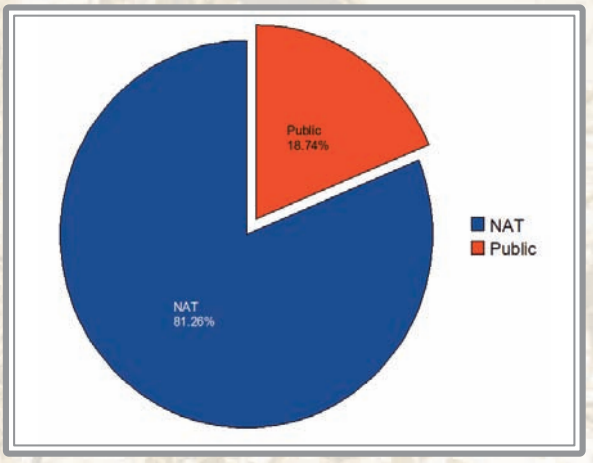


Figure 3. Efforts to assign private IP addresses to maximum number of clients continued.

The latest version of the OTRS system, used by our support staff, was placed into a live testing environment. As part of long-

term infrastructure planning, number of gigabit ports increased in comparison with the legacy 'FastEthernet' ports. (Figure 4).

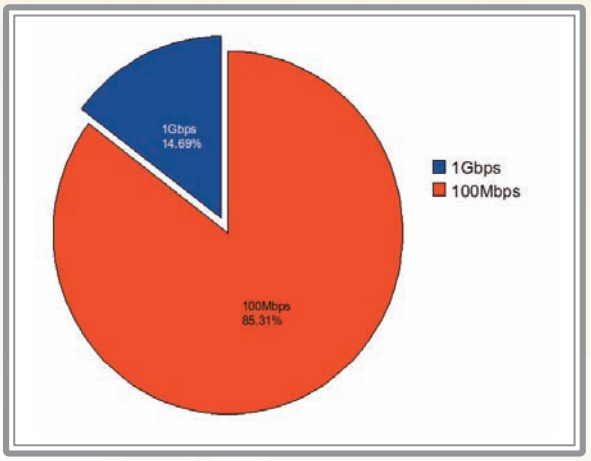


Figure 4. Network enhancement.

User support

Besides continuing support (as shown on Figure 5), the main project in this segment was creating the new help portal for users (http://helpdesk.irb.hr). This was motivated by the success of the old one, and modeled after similar knowledge bases composed elsewhere, bearing in mind technological and other trends.

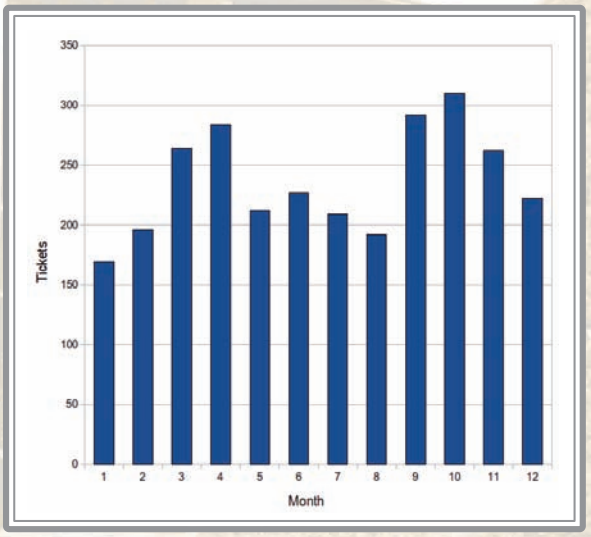


Figure 5. Help portal support.

CIR held an educational seminar (Figure 6) for our users with topics covering some of the newly provided services mentioned above and information security in general. This was also a good opportunity to discuss mutual needs and problems.

Figure 6. Education seminar about new services.

PROJECT INITIATIVES

In 2009 CIR prepared six EU FP7 project proposals for ICT Calls, with the aim to continue the eScience program orientation and to form the project chain in the line of eInfrastructure, distributed computing, parallel applications and scientific visualisation technologies.

EDUCATIONAL ACTIVITIES

CIR provides 5 undergraduate and 3 graduate courses at the Faculty of Electrical Engineering and Computing and at the Faculty of Graphical Arts of the University of Zagreb. In addition, CIR organized a workshop on 'High performance computing on Grid for meteo application, present cluster and grid technologies and WRF prognostic model' for the wider public with special focus on the meteorological community.

ORGANISATION OF CONFERENCES

CIR organized the annual Conference 'Grid and Visualisation Systems' as part of the

International Convention MIPRO in Opatija May 23-28, 2009 (http://www.mipro.hr/gvs.htm), as well as the 5th PSC meeting on 'SEE-GRID eInfrastructure for regional eScience' in Dubrovnik, September 9-11, 2009.

PROJECTS

Projects supported by Ministry of Science, Education and Sport

1. Scientific Visualisation Methods, Karolj Skala

Programs supported by the Ministry of Science, Education and Sports

1. Distributed Computing and Visualisation, Karolj Skala

Research, development and international projects

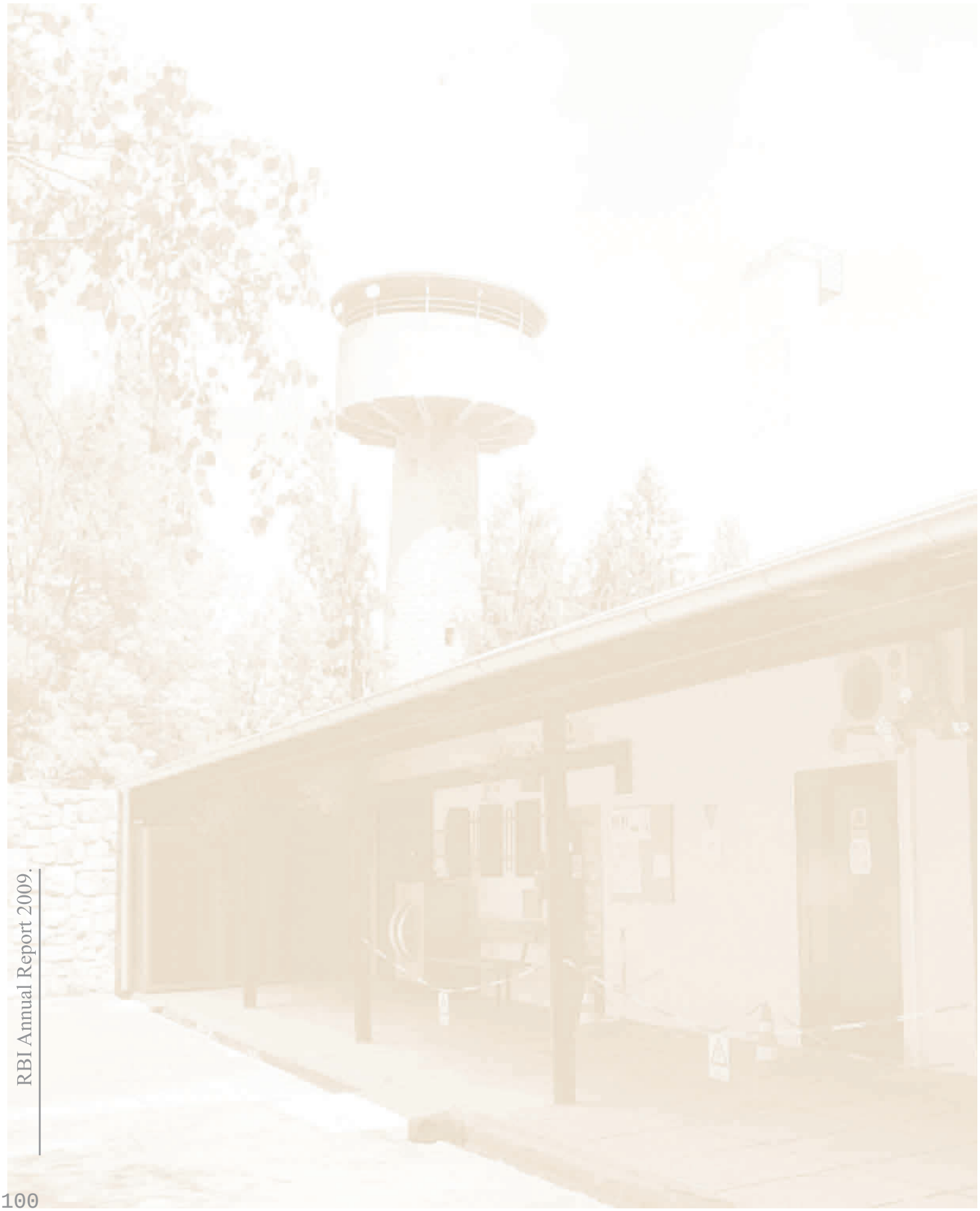
1. Enabling Grids for E-science-III (EGEE-III), Karolj Skala (EU FP7)
2. South Eastern European GRid-enabled eInfrastructure Development 2 (SEE GRID SCI), Karolj Skala (EU FP7)
3. Digital Research Infrastructure for the Arts and Humanities (DARIAH), Karolj Skala (EU FP7)

SCIENTIFIC SERVICE (SOFTWARE)

Protein data Base Graphic Generator http://mamlaz.irb.hr/pdb_grafika

SELECTED PUBLICATION

1. Poljak-Blaži M, Kolarić D, Jaganjac M, Žarković K, Skala K, Žarković N: Specific thermographic changes during Walker 256 carcinoma development: Differential infrared imaging of tumour, inflammation and haematoma. *Cancer detection and prevention* **32** (2009), 431.



Centre for Nuclear Magnetic Resonance

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

ORGANIZATION OF THE CENTRE

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

The Centre consists of the following laboratories:

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

Figure 1. Helium refilling of the 14 T magnet (Bruker 600 MHz).

OVERVIEW OF THE CENTER

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

In 2009, the members of the Center made valuable contributions to peptide and organometallic chemistry, photochemistry, biochemistry, solid state chemistry, and chemical graph theory and modelling. The scientists of the Center continued to be involved in lecturing at the Universities of Zagreb, Split, Osijek, Dubrovnik, and Rijeka, and organized a number of scientific conferences and courses. Active international collaborations were maintained.

TOP ACHIEVEMENTS

Non-linearity and frequency shifts of nuclear magnetic spin-noise

The lineshapes observed in proton nuclear spin-noise spectra, which depend in a complex way on the properties of the resonance circuit, the number of spins present, transverse relaxation, inhomogeneous broadening, and radiation damping were systematically investigated by high resolution ^{1}H noise power NMR spectra of liquid samples. Simulations based on an adapted Nyquist noise equation were used to understand and interpret the experimental findings (Nausner et al., 2009).

Assignation of NMR spectra of new compounds

Novel 1-(o-vinylphenyl)-4-(phenyl/2-furyl) butadienes were synthesized in one step via intramolecular photocycloaddition reaction. The photochemical products were characterized in $CDCl_3$ solution by different 1D- and 2D NMR techniques (Škorić et al., 2009).

A novel cobalt(II) complex of 3-methylpicolinic acid was prepared and characterized in solution by NMR spectroscopic methods. The N,O-chelated coordination mode of the ligand in the complex was confirmed (Kukovec et al., 2009).

Application of methods of discrete mathematics to various chemical problems

Using topological considerations, especially those based on the Wiener index, the relative stability, reactivity and the number of ^{13}C NMR resonance peaks as well as their relative intensities were derived for C_{28} fullerenes (Ori et al., 2009).

The sum-connectivity index was introduced and compared with well-known Randić product-connectivity index. It was shown that both indices correlate well among themselves and with the π-electronic energies of benzenoid hydrocarbons (Lučić et al., 2009).

A novel compact 2-D graphical representation of proteins based on the concept of virtual genetic code and a four-color map was proposed. The novel representation enables one to easily carry out a visual inspection of similarity/dissimilarity between proteins and it also leads to a numerical characterization of proteins (Randić et al., 2009).

Physiological effects of D- and L- enantiomes of melanocortin peptides *in vivo*

The hepatoprotective effects of the L- and D-enantiomers of α-melanocortin peptide (α-MSH) *in vivo* were investigated. L-α-MSH exhibited potent hepatoprotective effect in the experimental model of acetaminophen induced hepatotoxicity in male CBA mice, while its D-mirror image was inefficient (Turčić et al., 2009).

Frequency-dependent fluidity and conductivity of an ionic liquid

The frequency- and temperature-dependent shear fluidity of the ionic liquid, 1-butyl-3-methyl-imidazolium tetrafluoroborate - $[BMIm]BF_4$, was presented and compared with its ionic conductivity. Based on modelling of experimental results in terms of the MIGRATION concept it was concluded that the time correlation function for shear flow has significant features in common with the current density autocorrelation function (Šantić et al., 2009).

EDUCATION

In 2009, the members of the Center taught 5 undergraduate and 10 postgraduate courses at Universities in Zagreb, Split, Osijek, Dubrovnik, and Rijeka.

AWARDS

The Croatian State Annual Award for Science was given to Ante Graovac, senior scientist at the Center for NMR and Professor at the Faculty of Science, University of Split. Ante Graovac was awarded for discovery and development of novel methods of mathematical chemistry and their applications to various fields of chemistry and material sciences.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

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

Research, developmental and international projects

1. Multi-field experimental high resolution NMR studies with applications to bioactive compounds, Vilko Smrečki, (MSES, bilateral collaboration with Austria)
2. Applications of topological, geometric, algebraic and combinatorial methods in sciences, Ante Graovac (MSES, bilateral collaboration with Slovenia, No. 14).
3. New insights into charge transport in iron phosphate glasses from analysis of conductivity spectra over a wide temperature range, Andrea Moguš-Milanković (DAAD, bilateral collaboration with Germany)
4. Investigation of the frequency-dependent mechanical properties of polymer electrolytes, Ana Šantić (Postdoctoral project, SFB 458 and University of Münster, Germany)
5. Novel method to support bone growth bioactive glass coated with protein/lipid poroxidation products, Nationalbank Jubiläumsfonds Grant (Nr. 12611), LKH Graz, Renate Wildburger (Neven Žarković, Andrea Moguš-Milanković)
6. The origin of structural defects and their influence on macroscopic properties of solar silica glass, Davor Gracin, (Andrea Moguš-Milanković), (NFS Croatia, Ruđer Bošković Institute-Lipik Glas d.o.o.)

Contracts with industry

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

SELECTED INVITED LECTURES

1. Štambuk N. Perspectives and limitations of the molecular recognition theory. Clinical Institute of Laboratory Diagnosis, UHC Zagreb, February 18, 2009.
2. Moguš-Milanković A. Electrical properties of phosphate glasses. International Seminar on Science and Technology of Glass Materials, IS-STGM 2009, Nuzvid, India, March 16-20, 2009.
3. Graovac A. Shape analysis of carbon nanotube junctions. The Second Conference and Workshop on Mathematical Chemistry (SC-WMC 09), University of Kashan, Kashan, Iran, April 14-16, 2009.
4. Smrečki V. Isotope effects in NMR spectra of aromatic compounds with deuterium labelled phenyl ring. XXI Croatian Meeting of Chemists and Chemical Engineers, Trogir, Croatia, April 19-22, 2009.

SELECTED ORGANIZED CONFERENCES AND COURSES

1. Algebraic Graph Theory 2009, Dubrovnik, Croatia, June 01-07, 2009., organized by A. Graovac

2. MATH/CHEM/COMP 2009, The 24th International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences. Dubrovnik, Croatia, June 08-13, 2009., organized by A. Graovac, P. Konjevoda, D. Plavšić, V. Smrečki, D. Vikić-Topić, M. Vinković

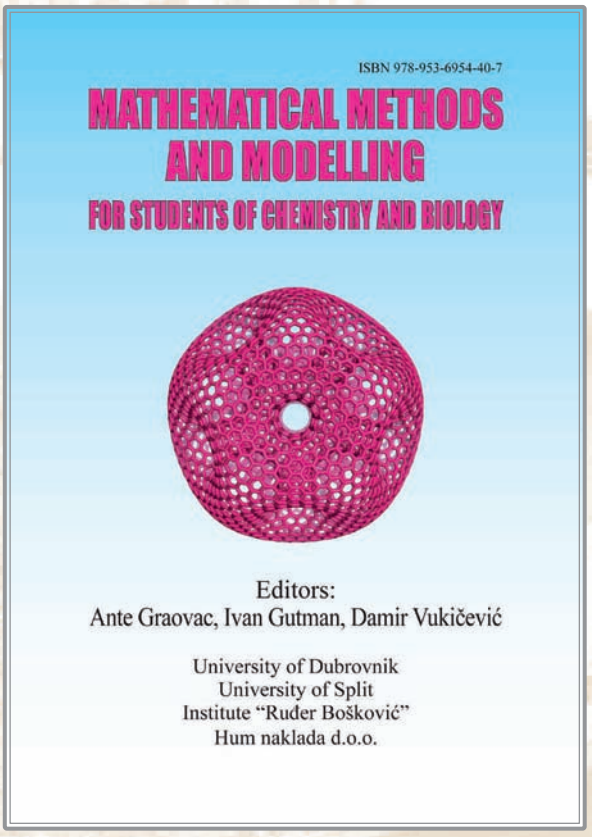


Figure 2. This book is intended to serve as additional literature for students of chemistry, biology, biophysics, and mathematics.

SELECTED PUBLICATIONS

Research articles

1. Nausner M, Schlagnitweit J, Smrečki V, Yang X, Jerschow A, Müller N: Nonlinearity and frequency shifts of nuclear magnetic spin-noise. *J Magn Reson* **198** (2009), 73.
2. Škorić I, Šmehil M, Marinić Ž, Molčanov K, Kojić-Prodić B, Šindler-Kulyk M: Photochemistry of ω-(o-vinylphenyl)-ω'-(phenyl/2-furyl) butadienes: New approach to 4- substituted benzobicyclo[3.2.1]octadienes. *J Photochem Photobiol A Chem* **207** (2009), 190.
3. Kukovec B-M, Popović Z, Komorsky-Lovrić Š, Vojković V, Vinković M: Synthesis, structural, spectroscopic and thermal characterization of cobalt complexes with 3- and 6-methylpicolinic acid. Voltammetric and spectrophotometric study in solution. *Inorg Chim Acta* **362** (2009), 2704.
4. Ori O, Cataldo F, Graovac A: Topological ranking of C_{28} fullerenes reactivity. *Fuller Nanotub Car N* **17** (2009), 308.
5. Lučić B, Trinajstić N, Zhou B: Comparison between the sum-connectivity index and product-connectivity index for benzenoid hydrocarbons. *Chem Phys Lett* **475** (2009), 145.
6. Randić M, Mehulić K, Vukičević D, Pisanski T, Vikić-Topić D, Plavšić D: Graphical representation of proteins as four-color maps and their numerical characterization. *J Mol Graph Modell* **27** (2009), 637.
7. Turčić P, Bradamante M, Houra K, Štambuk N, Kelava T, Konjevoda P, Kazazić S, Vikić-Topić D, Pokrić B: Effects of α-melanocortin enantiomers on acetaminophen-induced hepatotoxicity in CBA mice. *Molecules* **14** (2009), 5017.
8. Šantić A, Wrobel W, Mutke M, Banhatti RD, Funke K: Frequency-dependent fluidity and conductivity of an ionic liquid. *Phys Chem Chem Phys* **11** (2009), 5930.

Book chapters

1. Vukičević D, Graovac A (2009) Comparison of the M1 and M2 indices. Overview of the results. In: Mathematical methods and modelling for students of chemistry and biology - Editors: Graovac, A, Gutman I, Vukičević D, Hum naklada d.o.o., Zagreb 2009, pp 133-141.

Books

1. Mathematical methods and modelling for students of chemistry and biology (Graovac A, Gutman I, Vukičević D. eds). Hum naklada d.o.o., Zagreb 2009.

Library

http://library.irb.hr

LIB

Head of Library: Jadranka Stojanovski
(until February 28th 2009)
Bojan Macan (from November 20th 2009)

GOALS AND OBJECTIVES

In the last decade the library world has witnessed evidence of the global crisis in the scholarly publishing sphere. The majority of the RBI Library activities were focused on overcoming the gap between the conservative and old fashioned format of scholarly publications favoured by the influential commercial publishers, and the needs and demands of library users to access the literature more freely and in an easy and simple way. Recognizing the open access movement as the only path which will lead to the development of scholarly publishing in the future, the Library was the main initiator of numerous activities related to the open access movement and easier access to journals and other publications, in keeping with global trends.

Along with the problem of access to literature, and keeping in mind that the number of publications is growing exponentially, there is constant pressure to select those publications which are the most influential and have the highest quality in the field. This selection relies on subjects such as bibliometrics, which reflects the development of different criteria for the evaluation of scholarly publishing. Though controversial and often misinterpreted by researchers, bibliometrics indicators have become increasingly important in the RBI research community. Bibliometric measures, properly used and interpreted, may characterize aspects of research productivity and influence. With their expertise in the field, librarians are assisting RBI management to utilize bibliometric indicators in assessing the Institute and its departments, laboratories and research projects domestically and internationally. To individual researchers the use of bibliometric indicators, such as number of published papers and their citations, *h*-index, and other indicators, can help in promotions and career development.

OVERVIEW OF LIBRARY ACTIVITIES

In 2009 the Library focused on a few important projects. First of all, was completion of the implementation of the integrated library system – Koha and release of its production version. This implementation was a very important segment in the future plans for modernization of the Library's management system and providing modern, high quality services to the Library's users. After more than a year of hard work on implementation and conversion of metadata from the UNIMARC to the MARC21 standard, the RBI Library has finally released Koha into the production phase. The RBI's database of books was converted and imported into

Koha, RBI's user database was created by connecting with the local LDAP database and circulation of books was computerized. Koha is now used for acquisition, cataloguing and circulation of books. Along with implementation of Koha, the new Online Public Access Catalogue was also implemented (https://katalog.irb.hr/).

A second important project for the RBI Library, as well as for the Institute itself, was implementation of RBI's digital repository. In 2009 most of the Library's efforts went toward digitalization of photographic and other documentary materials and its organization and preparation for future archiving in a digital repository. Around 6,000 old photographs were digitized and organized, as well as one part of old reports and annual reports. Release date of the RBI's digital repository is expected to be in 2010.

Last but not least, was the project to build a database of comprehensive bibliography of RBI's papers, together with their citations from the Web of Science database. The database was improved, with the addition of a few additional features and the data on published papers, their citations and RBI scientists were updated. On the basis of this database, a number of bibliometric analyses were performed for a variety of purposes. In addition to working on this database, the Library's staff provided a number of bibliometric analyses to individual RBI scientists and Institute management.

COLLECTIONS

Digital collection

In 2009, there were around 16,000 fee and free e-journals available to the Croatian academic community. This decrease in total number of available journals occured because in 2009 the Ministry of Science, Education and Sports did not re-new subscriptions with the major publishers (Springer, Blackwell, Nature Publ. etc.). On the other hand, RBI subscribed to an additional 54 e-journals published by smaller but no less important publishers. Access to the available e-journals was provided via an in-house developed search engine of e-journals – Pero (http://knjiznica.irb.hr/pero/). Through the Centre for Online Databases (http://www.online-baze.hr/), there were also around 30 free and fee biomedical and natural sciences databases, as well as 42 e-books available to RBI researchers.

Printed collection

Although the RBI library can be characterized as a *digital library* and it provides most of its collections online in digital form, printed collections still play an important role in scientific communication among RBI researchers. RBI's printed book collection amounts to 22,518 volumes, 345 of which were newly acquired in 2008. In addition to the e-journals collection available to RBI researchers, 69 print subscriptions were available.

Figure 1. The new RBI Library's OPAC

SERVICES

The RBI Library web site has become a starting point for the RBI researcher's quest for relevant information. It consists of many web pages, organized digital collections and services and because of its usefulness it is very popular among the whole Croatian academic community (in the year 2009 it has averaged over 200,000 visits per month).

Figure 2. RBI Library's Facebook account

In the year 2009, the RBI Library has developed a few new services as well as maintaining a number of existing services and projects, both for RBI users and the whole Croatian academic community. These services make access to relevant information easier and a few of these services and projects are listed here:

- OPAC – Online Public Access Catalogue (https://katalog.irb.hr)
- Facebook group – Knjižnica Instituta "Ruđer Bošković" (http://www.facebook.com)
- Library Blog (http://knjiznica.irb.hr/blog/)
- SEND - Interlibrary Loan Service (http://send.irb.hr)
- Pero – Search engine of e-journals (http://knjiznica.irb.hr/pero/)
- IRB reservations (developed with Centre for Informatics and Computing) (https://rezervacije.irb.hr/)
- CROSBI – Croatian Scientific Bibliography (http://bib.irb.hr)
- Who's Who in Croatian Science (http://tkojetko.irb.hr)
- Centre for online databases (http://www.online-baze.hr)
- CMS for web sites of Croatian academic and research libraries (http://knjiznice.szi.hr)
- Hrčak – Portal of Scientific Journals of Croatia (http://hrcak.srce.hr/).

Figure 4. RBI Library's Blog

The Library also continued to organize the regular RBI Library Colloquia. Through monthly lectures and presentations RBI hosted librarians and information specialists from different academic, specialty and public libraries. Colloquia topics were chosen to be of interest not only to librarians, but also to RBI staff and the general public.

Interlibrary loan

The RBI library has a well established interlibrary loan and lending service with libraries from Croatia and abroad. In 2009 the RBI library received 925 requests for document delivery by RBI staff and 922 of those requests were positively resolved. As well, the RBI library also received 448 requests for document delivery from other Croatian libraries, and positively resolved 402 of those requests. Interlibrary loan services from other libraries from Croatia are mainly free of charge, while documents from libraries from abroad carry a small charge. However, in 2008 the RBI library established a successful collaboration with the IAMSLIC organization wherein members can obtain interlibrary loans free of charge. In 2008 there were 187 documents acquired from IAMSLIC libraries free of charge, and this was the second most used source for document ordering, right behind the commercial Subito source (catalogue of German libraries).

EDUCATION

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

MEMBERSHIPS

The Library continued its international collaboration with EURASLIC (European Association of Aquatic Sciences Libraries and Information Centres) and its parent organisation IAMSLIC (European Association of Aquatic Sciences Libraries and Information Centres). These associations link together aquatic sciences libraries and information centres with the intent to undertake joint projects, to improve the flow, exchange and dissemination of aquatic information. The Library also had an active role in EURASLIC activities, with two of its members on the EURASLIC board, as well as in the subgroups ECET (European Countries in Economic Transition) and MedSig (The Mediterranean Special Interest Group). Library staff also participated in training courses held at UNESCO/IOC Project Office for IODE in Oostende, Belgium. In 2009 two grants for training course were received:

- Training Course on website development, June 15th-June26th, 2009
- The Digital Asset Management (DAM) Workshop, October 2nd-7th, 2009

Library staff also participated at The 35th IAMSLIC Annual Conference & 13th Biennial EURASLIC Conference held in Brugge, Belgium from September 27th - October 1st, 2009.

SELECTED LECTURES

1. Vodopijevec A, Macan B. Implementation of digital repository at the Ruđer Bošković Institute: organizational and technical issues title of lecture. The Future of Information Sciences: INFuture2009: Digital Resources and Knowledge Sharing, Zagreb, Croatia, November 4-6, 2009.
2. Stojanovski J. Technology implementation trends in libraries. 9th annual conference of the Croatian academic and scientific libraries: The library strikes back: Reorganizing the empire, Zagreb, Croatia, November 13-14, 2009.
3. Macan B. The criteria for evaluation of scientific journals: advantages and disadvantages. 9th annual conference of the Croatian academic and scientific libraries: The library strikes back: Reorganizing the empire, Zagreb, Croatia, November 13-14, 2009.
4. Konjević S, Mayer M. What's New @ RBI Library. The 35th IAMSLIC Annual Conference and 13th Biennial EURASLIC Conference, Brugge, Belgija, September 27 – October 1 2009.

CONFERENCE ORGANIZATION

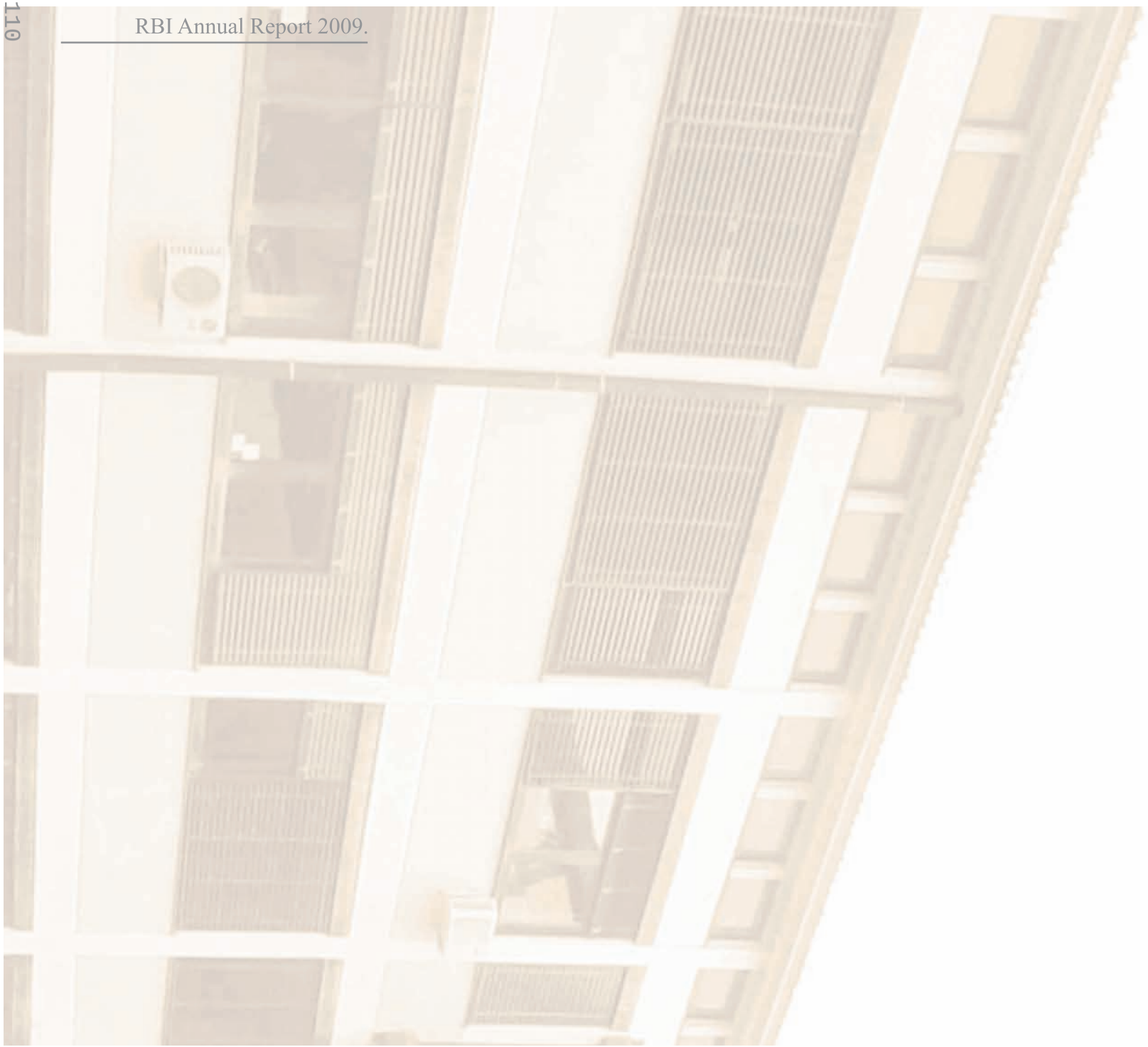
Figure 3. Librarian's 2009 conference with reorganizing the services as main topic

The 9th annual conference of Croatian academic and specialty libraries entitled "The library strikes back: Reorganizing the empire" was organized by the Croatian Academic and Research Network CARNet, Faculty of Electrical Engineering and Computing philosophy, Faculty of Humanities and Social Sciences and the RBI Library at the Faculty of Electrical Engineering and Computing, University of Zagreb, Zagreb, from November 13-14, 2009.

Figure 5. IAMSLIC/EURASLIC Conference participants (photography taken by Misjel Decleer)

SELECTED PUBLICATIONS

1. Stojanovski J, Petrak J, Macan B: The Croatian national open access journal platform. *Learned Publishing* **22** (2009), 263.
2. Macan B: Web 2.0 technologies and their use in libraries - experience of the Ruđer Bošković Institute Library with especial addition to Library Blog. *Chem Industry* **58** (2009), 226.
3. Pažur Vojvodić I: Has the acces increased? Chemisty in industry - website access analysis 2007 and 2008. *Chem Industry* **58** (2009), 270.
4. Konjević S: SEND - System of electronic document delivery. *Chem Industry* **58** (2009), 130.
5. Pažur Vojvodić I: Zotero – bibliografic management program. *Chemistry Industry* **58** (2009), 345.
6. Macan B: The new OPAC of the Ruđer Bošković Institute Library. *Chemistry Industry* **58** (2009), 10-464.



Rudjer Innovations Ltd.

http://www.r-i.hr

COMPANY ORGANIZATION

Head of Management Board:
Domagoj Oreb, CEO

Member of Management Board:
Dinko Smolčić, CFO

Member of Management Board:
Božidar Etlinger

Business Development Manager:
Davor Aničić

Business Development Manager:
Davorka Moslavac-Forjan

Business Development Manager:
Lidija Stopfer

Project Analyst: Matea Novosel

OVERVIEW OF THE COMPANY

Rudjer Innovations LLC is a company specialised in the commercialisation of innovations and technology transfer. It links science and technology to the economy and industry. The company addresses the needs of the scientific community, both researchers and innovators, assisting them in the commercialisation of inventions and scientific research results, as well as assisting companies that are willing to apply the know-how of the scientific community in their business operations. Rudjer Innovations was founded with the full support of the Croatian Government and the World Bank as a daughter company of the Ruđer Bošković Institute. The mission of Rudjer Innovations is to contribute to the development of Croatia as a knowledge based society by linking the scientific and research community with enterprises and businesses and thus through commercialisation of knowledge strengthen the competitiveness of Croatia in the global market. The goal of Rudjer Innovations is to establish cooperation which brings together the mutual interests of science and business, ensuring a win-win result, with numerous competitive advantages for both companies and scientists. The activities of Rudjer Innovations include: identification and evaluation of research results and inventions; protection of intellectual property and assistance in selecting and implementing an appropriate commercialization model (licensing, establishing spin-off companies, joint ventures). Rudjer Innovations also provides consultancy services for technology transfer and business agreements, as well as financial support for innovations and projects.

ACHEIVEMENTS IN 2009

Portfolio

The portfolio of Rudjer Innovations contains more than 80 inventions and R&D projects with commercial potential in various fields including primarily chemistry, medicine, biology, physics and informatics. Some have already been applied in industry and the economy, and others have been prepared for various methods of commercialisation, depending on the interests and needs of the respective partners. In addition to its portfolio of innovations, Rudjer Innovations works on strengthening cooperation between the Ruđer Bošković Institute and companies from various business areas. Ruđer Bošković Institute's know-how, professionalism and multidisciplinary approach in solving problems in various areas represents a great resource for cooperation with companies.

PATENTS

Two patents of Ruđer Bošković Institute were granted in 2009; one European patent (EP 1786763 "NNN-Tris-(3-dimethylaminopropyl)-guanidine, the procedure of preparation from carbodiimide and application in reactions of transesterification of oil", M. Maksić, Z. Glasovac) and one United States patent (No. 7,658,850 "Mixed bacterial culture for atrazine degradation", D. Hršak, M. Havriluk).

Rudjer Innovations filed 6 new patent applications on behalf of the Ruđer Bošković Institute in 2009 - 5 Croatian national applications and 1 international patent application). Furthermore, 3 existing Croatian national patent applications entered the international (PCT) phase in 2009 and 6 patent applications were filed in the national phase of patent protection in 2009 (two in the EU, three in the USA and one in Canada).

AWARDS

Rudjer Innovations LLC participated at the International Fair of Innovations, New Ideas, Products and Technologies ARCA 2009 and presented inventions of Ruđer Bošković Institute. The company received the following awards:

1. Plaquette ARCA 2009 for participation
2. Silver Arca for innovation "Preparation of percipitated calcium carbonate (PCC) in semi continuous process" (D. Kralj, Rudjer Bošković Institute)

ACTIVITIES AND PROJECTS

Within its commercialisation activities, Rudjer Innovations continued building its network of contacts with business and industry in Croatia and internationally, which resulted in the initiation of several licensing and business cooperation negotiations in 2009. It signed a business cooperation agreement with the US intellectual property brokerage company, which improved the company's international reach and raised interest in Rudjer Innovations' portfolio.

The company evaluated several proposals for spin-off companies and participated in the preparation of a new spin-off company for the commercialisation of an electrostatic modelling method developed in the Theoretical Physics Division of the Ruđer Bošković Institute. Rudjer Innovations also co-developed a new business model for an existing spin-off company at the Ruđer Bošković Institute, Biozyne LLC.

Rudjer Innovations assisted the Ruđer Bošković Institute in finding industry partners and applying for several R&D projects through the Croatian Business Innovation Centre (BICRO), one of which was awarded in 2009. The company became a member of the American Chamber of Commerce and British Croatian Business Network. Furthermore, it supported creation of the Croatian

Business Angel Network (CRANE), the first of its kind in Croatia.

Rudjer Innovations took part in the PHARE project "Capacity building in technology transfer institutions in order to enhance research commercialization activities" administered by the Ministry of Science, Education and Sports, aimed at supporting emerging technology transfer activities in Croatia. With its local and international partners, the company also applied for several EU funded projects, both national (IPA) and transnational (SEE). It became a member of the Association of European Science and Technology Transfer Professionals (ASTP) and of the Enterprise Europe Network (EEN).

Within the areas of promotion and strengthening of science and industry cooperation, Rudjer Innovations participated in a number of events organized by both the public and private sector, both national and international. These events included:

- National Innovation System Conference (speaker), Ministry of Science, Education and Sports, Croatia
- Technology Transfer Conference (speaker), Jozef Stefan Institute, Slovenia
- VIDI e-novation award for high-tech innovations (co-organizer), Croatia
- Private Equity & Venture Capital round table (speaker), Croatia
- "Round table: Protection of intellectual property: precondition for development of Croatian economy?"(speaker), WinDays 2009 Microsoft Conference, Croatia
- "SME Week"(speaker). Croatian Business Innovation Centre, Croatia

The Rudjer Innovations database of inventions, projects and spin-off companies is available at www.r-i.hr