

4th European Conference on Chemistry for Life Sciences (4ECCLS)
August 31 – September 3, 2011 Budapest, Hungary

Summary for ESF Euroglycoforum Grant
Science meeting 3358

The **4th European Conference on Chemistry for Life Science (ECCLS)** was held 31 August -3 September 2011 in Budapest, Hungary. Previous conferences were held in Rimini (2005), Wroclaw (2007) and Frankfurt (2009). The Budapest Conference inspired an interdisciplinary audience and attracted young researchers to this nascent and highly flourishing field of chemistry and biology.

The conference was a great success, there were closely **400 participants (154 students)** from **37 countries**, of **4 continents** on the event. The organizers invited leading scientists of the field, **5 plenary** (Ivano Bertini, Bernt Krebs, Wolfgang Lubitz, Dieter Seebach, Julio M. Fernandez) and **11 keynote** (Roger Alberto, Andrea Bodor, Imre G. Csizmadia, Dieter Enders, Ernst Giralt, Charlotte Hauser, Ole Hindsgaul, Henryk Kozlowski, Paul D. Leeson, Sheref S. Mansy, Bengt Nordén) speakers.

Moreover there were **89 oral presentations** delivered and **171 poster presentations** on view in **15 sessions**: The Conference covered a wide, interdisciplinary and intersectorial field. With its numerous topics from bioorganic chemistry to bioinorganic chemistry, from chemical biology to structural biology, from glycochemistry to the nucleic acid chemistry, from the chemistry of the „omes” to bionanomaterials, etc. it brings together scientists from different disciplines to find answers to their common questions how chemistry can help to answer their questions concerning details or essence of some life process. These conferences can be very flourishing, as we experienced so far during the past events of this series.

This year a 4 parts Tutorial (towards biology) complemented the Conference for non specialist who wanted to get some medium-level knowledge and skill in molecular biology and molecular biological methods.

Undoubtedly, the Conference was a great success and evidenced by the attendance and the quality of presentations. The next meeting is awaited eagerly with great anticipation and will be held at the University of Barcelona in Spain between June 10-12, 2013.

The conference webpage is accessed at www.4eccls.mke.org.hu.

Budapest, 21. October 2011.

Beáta Androsits
Hungarian Chemical Society

Description of the scientific content of the Conference and discussion at the event

The Hungarian Chemical Society proposing is organized the **4th European Conference on Chemistry for Life Sciences (4ECCLS)** in Budapest, Hungary. This Conference was held at Congress Centre of Eötvös Lóránd University is located in the centre of the capital, at the riverside of the Danube. The Congress Centre of Eötvös Lóránd University is well equipped for large-sized conferences. It has large lecture halls with excellent equipments, space for posters sections and sufficient catering facilities for the participants. The Hungarian Chemical Society generally organizes 10-15 scientific conferences (international and hungarian) yearly. The conference administration was handled by the Hungarian Chemical Society too.

Scientific Committee:

Thomi Brunner Switzerland, Huub de Groot Netherland, Julio Fernandez United States, Nick Hadjiliadis Greece, Knud J. Jensen Denmark, Matthias Kaestner Germany, Tamás Kiss Hungary (Chairman of Organizing Committee), Robert Konrat Austria, Henryk Kozlowsky Poland, Stefan Oscarsson Ireland, Claude F. Meares United States, Sven Panke Switzerland, András Perczel Hungary (Chairman of Organizing Committee), Janez Plavec Slovenia, Michael Przybylsky Germany, Peter Schreiner Germany, G. Matthias Ullmann Germany.

Local Organizing Committee:

Tamás Kiss (University of Szeged)
András Perczel (Eötvös Lóránd University) (Chairs of the conference)
Beáta Androsits and Mónika Bondár (Hungarian Chemical Society).

List of invited plenary speakers:

Ivano Bertini (University of Florence, Italy)
Bernt Krebs (University of Muenster, Insititute of Inorganic and Analytical Chemistry, Germany)
Wolfgang Lubitz (Max-Planck Institut für Bioorganische Chemie, Germany)
Dieter Seebach (ETH Zürich, Organic Chemistry and Applied Biosciences, Germany)
Julio M. Fernandez (Columbia University, Biological Sciences, NY. USA)

List of keynote speakers:

Roger Alberto (University of Zürich, Inorganic Chemistry, Switzerland)
Andrea Bodor (Eötvös Lóránd University, Department of Analytical Sciences, Hungary)

Imre G. Csizmadia (University of Szeged, department of Chemical Informatics, Hungary)

Dieter Enders (RWTH Aachen University, Institute of Organic Chemistry, Germany)

Ernst Giralt (Institute for Research in Biomedicine (IRB), Spain)

Charlotte Hauser (Institute of Bioengineering and Nanotechnology, Singapore)

Ole Hindsgaul (Carlsberg Laboratory, Denmark)

Henryk Kozlowski (University of Wroclaw, Faculty of Chemistry, Poland)

Paul D. Leeson (AstraZeneca, R&D Charnwood, Respiratory and Inflammation, UK)

Sheref S. Mansy (University of Trento, CIBIO, Italy)

Bengt Nordén (Chalmers University of Technology, Physical Chemistry, Sweden)

Conference program. 45 min plenary lectures, 25+5 min keynote lectures, 15+5 oral communications,

Date/time	9:00-11:30	11:40-13:00	13:00-14:00	14:00-15:40	16.00-19.00	19:00
		Registration	Registration	Registration Tutorial	16.00 opening ceremony, 17.00 plenary lecture	Get-together party
Sept 1. four parallel session	Oral Session	Oral Session Tutorial	lunch	Oral Session Tutorial	Poster Session	Organ Concert
Sept 2. four parallel session	Oral Session	Oral Session Tutorial	lunch	Excursion	To Visegrad	Banquet
Sept 3. four parallel session	Oral Session	Oral Session and closing ceremony	lunch			

The conference program consisted of plenary lectures (invited), session lectures (keynote), oral presentations (selected from Abstracts) and poster sessions., banquet.

Four Tutorials were held: (1. Macromolecular Interactions, 2. Essential Gene Technology for Chemists, 3. How living cells work: structure and function, 4. 21 st-Century Enzymology)

The conference included 5 plenary lectures and 11 keynote lectures. The scope of the conference was very broad covered 15 different topics of interdisciplinary fields between chemistry, biology, medicine, etc.

Many of young researchers attended on the event, from the **154 students** 36 of them got **ESF student grants** from (ESF Student Grant - supported by Euroglycoforum). The acceptance was made by Prof. Tamás Kiss and Prof. András Perczel (Chairs of 4. ECCLS Conference).

Examples of major topics of the conference:

Peptide/protein,

Bioconjugates,

Dynamics in Biology,

Computational Aspects of Biomolecules,

Glycochemistry,

Biomolecules in 3D,

Bioinorganic Chemistry,

Bioinspired Organocatalysis,

Bio-nanotechnology,

Neurochemistry and Neurodegenerations,

Frontiers in Medicinal Chemistry,

Nucleic Acids,

Metals in medicine,

Artificial Photosynthesis,

Biogeochemistry

One of them was devoted to Glycochemistry - Glycoscience. The topic was organised and chaired by an international and a „local” outstanding representative scientists of the research field: Professors **Stefan Oscarsson** from Ireland and **Laszlo Somsák** from Hungary. Beside a keynote lecture 7 oral contributions and 26 poster presentations was included in the scientific programme of the Section.

This was one of the strongest sections.

O. Hindsgaul (Carlsberg Laboratory, Copenhagen, Denmark): Probing the biological functions of carbohydrates using small synthetic molecules (keynote)

In this lecture the speaker gave a short survey on the methods used in the analysis of carbohydrates, emphasising that the reliability of these techniques mostly depends on the availability of reference standards and the skilled application of the instrumental techniques such as 2,3-D NMR and MS. Then he focused on two simple chemistry-based methods developed in their laboratory, which need only a minimal use of sophisticated instrumental

methods. These were: 1) Fluorescent tagging of oligosaccharides using a new generation of „GlycanTips”, 2) Monitoring glycolipid metabolism in single human cells.

G.K. Gomba (Institute of Chemical Technology Prague, Czech Republic): Sugar composition and linkage analysis of fungal polysaccharides

K.J. Jensen (University of Aarhus, Denmark): Glycobiology of plant-microbe interactions

E.D. Chrysina (Institute of Organic and Pharmaceutical Chemistry, Athens, Greece): Structure-based inhibitor design of glycogen phosphorylase – an interdisciplinary approach for the treatment of type 2 diabetes

M. Czugler (Chemical Research Center, Budapest, Hungary): Sodium-sugar cotransport structure models

Y.-H. Tsai (Max Planck Institute of Colloids and Interfaces, Potsdam, Germany): Synthesis of Glycosylphosphatidylinositol-anchored protein

A. Borbás (University of Debrecen, Hungary): Sulfonic acid analogues of antithrombin-binding domain of heparin

P. Fügedi (Chemical Research Center, Budapest, Hungary): Towards stereoselective glycosylations: a critical tool for glycobiology

Valuable **poster prizes** were awarded to four young scientists by NJC (New Journal of Chemistry) and RSC (Royal Society of Chemistry). The winners in detail:

P9. Petros V. Gkazonis, Dionysios Vourtsis, Georgios A. Dalkas, Christos T. Chasapis, D. Bentrop, G.A. Spyroulias (Greece) A solution nmr study of native and mutated forms of the anthrax lethal factor catalytic site polypeptide

P142. Árpád Csog, Boldizsár Nagy, Kornélia Majdik (Romania) Heavy metal phytoaccumulation by aquatic plants (cabomba aquatica, vallisneria spiralis, echinodorus cordifolius)

P160 A. Czene, B. Gyurcsik, E. Endreffy and K. Nagata (Hungary) Novel diagnosis of duchenne muscular dystrophy

P180 B. Feng, F. Westerlund, B. Nordén (Sweden) DNA strand exchange catalyzed by polyethylene glycol

For more details of the 4th European Conference on Chemistry for Life Sciences visit the conference website at: <http://www.4eccls.mke.org.hu>

Budapest, 21. October 2011.

Beáta Androsits
Hungarian Chemical Society

Assessment of the results and impact of the event on the future of the field

The ECCLS conference series has a strategic impact on science in two respects. First, it covers an important, fast growing interdisciplinary field (chemistry in life sciences) and second, it brings together scientists from different fields: chemists from one side and others who want to apply the results of chemistry or need the help of chemists (sometimes they even do not know) to get answer to their questions. In this area of the European Community still has a pioneering role.

The Conference covers a wide, interdisciplinary and intersectorial field. With its numerous topics from bioorganic chemistry to bioinorganic chemistry, from chemical biology to structural biology, from Glycochemistry to the Nucleic Acid Chemistry, from the chemistry of the „omes” to Bionanomaterials, etc. it brings together scientists from different disciplines to find answers to their common questions how chemistry can help to answer their questions concerning details or essence of some life process. These conferences can be very flourishing, as we experienced so far during the past events of this series.

This year a 4 parts Tutorial (towards biology) complemented the Conference for non specialist who wanted to get some medium-level knowledge and skill in molecular biology and molecular biological methods. It was fairly popular students attended the course, who, at the end received a Certification about the participation.

This ESF Glycoscience Forum grant gave possibility to invite 36 young researchers to attend on the conference and presented their results. The student grant form ESF was especially useful to help training a new generation of young scientists.

Undoubtedly, it was a great success and evidenced by the attendance and the quality of presentations. The next meeting is awaited eagerly with great anticipation and will be held at the University of Barcelona in Spain between June 10-12, 2013.

Budapest, 21 October 2011

Beáta Androsits
Hungarian Chemical Society

Wednesday, 31 August 2011		
10:00 – 16:00	Registration	(Eötvös Loránd University, Budapest, Pázmány Péter sétány 1/A; Entrance from the river side)
13:00 – 16:00	Tutorials Towards Biology Tutorial 2: <i>Macromolecular interactions</i> Instructor: József Kardos (ELTE, Dept. Biochemistry)	(0.87 Marx Hall)
16:00 – 17:00	Opening ceremony	(-1.75 Conference Hall)
17:00 – 17:45	Ivano Bertini	Plenary Lecture (-1.75 Conference Hall)
17:45 – 18:30	Dieter Seebach	Plenary Lecture (-1.75 Conference Hall)
18:30 – 20:30	Get-together party	(1st floor, adjacent to the Spherical Hall)

Thursday, 1 September 2011				
9:00 – 9:45	Bernt Krebs		Plenary Lecture (-1.75 Conference Hall)	
Parallel sessions:				
	<i>(0.89 Jedlik Hall)</i>	<i>(-1.75 Conference Hall)</i>	<i>(0.81 Ortway Hall)</i>	<i>(0.83 Eötvös Hall)</i>
	PEPTIDE/PROTEIN BIOCONJUGATES	DYNAMICS IN BIOLOGY	COMPUTATIONAL ASPECTS OF BIOMOLECULES	GLYCOCHEMISTRY
9:50 – 10:10	Sarmay, Gabriella	Horváth, Gergő	Zaric, Snezana	Gomba, Gordon K.
10:10 – 10:30	Taki, Masumi	Arora, Rohit	Chaloin, Laurent	Jensen, Knud J.
10:30 – 10:50	Zawada, Zbigniew	Pires, Ricardo H.	Wieninger, Silke A.	Chrysina, Evangelia
10:50 – 11:10	Austen, Brian M.	Horn, Anselm H. C.	Iorga, Bogdan I.	Czugler, Mátyás
11:10 – 11:30 Coffee Break (<i>Ground floor, adjacent to the Spherical Hall</i>)				
Parallel sessions:				
	<i>(0.89 Jedlik Hall)</i>	<i>(-1.75 Conference Hall)</i>	<i>(0.81 Ortway Hall)</i>	<i>(0.83 Eötvös Hall)</i>
	PEPTIDE/PROTEIN BIOCONJUGATES	DYNAMICS IN BIOLOGY	COMPUTATIONAL ASPECTS OF BIOMOLECULES	GLYCOCHEMISTRY
11:30 – 12:00	Hauser, Charlotte	Harami, Gábor	Csizmadia, Imre G.	Hindsgaul, Ole
12:00 – 12:20	Boisguerin, Prisca	Lakatos, Andrea	Miscione, G. P.	Tsai, Yu-Hsuan
12:20 – 12:40	Nokihara, Kiyoshi	Batta, Gyula	Beke-Somfai, Tamás	Borbás, Anikó
12:40 – 13:00	Els, Sylvia	Rovó, Petra	Kozma, Daniel	Fügedi, Péter
10:00 – 13:00	Tutorials Towards Biology Tutorial 3: <i>Essential gene technology for chemists</i> Instructor: László Nyitray (ELTE, Dept. Biochemistry)			<i>(0.87 Marx Hall)</i>
13:00 – 14:50 Lunch (<i>First floor, adjacent to the Spherical Hall</i>)				
Parallel sessions:				
	<i>(0.89 Jedlik Hall)</i>	<i>(-1.75 Conference Hall)</i>	<i>(0.81 Ortway Hall)</i>	<i>(0.83 Eötvös Hall)</i>
	PEPTIDE/PROTEIN BIOCONJUGATES	BIOMOLECULES IN 3D	BIOINORGANIC CHEMISTRY	BIOINSPIRED ORGANOCATALYSIS
14:50 – 15:20	Bodor, Andrea	Delepierre, Muriel	Kozłowski, Henryk	Enders, Dieter
15:20 – 15:40	Mező, Gábor	Pál, Gábor	Árus, Dávid	Jordan, Frank
15:40 – 16:00	Ahrens, Verena M.	Plavec, Janez	Ha Duong, Nguyet-Thanh	Tárkányi, Gábor
16:00 – 16:20	Láng, Júlia A.	Nyitray, László	Rowinska-Zyrek, M.	Schmidtchen, Franz
16:20 – 16:40	Pipkorn, Ruediger	Viskolcz, Béla	Gumienna-Kontecka, E.	Lionne, Corinne
16:40 – 17:00 Coffee Break (<i>Ground floor, adjacent to the Spherical Hall</i>)				
Parallel sessions:				
	<i>(0.89 Jedlik Hall)</i>	<i>(-1.75 Conference Hall)</i>	<i>(0.81 Ortway Hall)</i>	<i>(0.83 Eötvös Hall)</i>
	BIO-NANOTECHNOLOGY	NEUROCHEMISTRY AND NEURODEGENERATION	BIOINORGANIC CHEMISTRY	BIOINSPIRED ORGANOCATALYSIS
17:00 – 17:20	Jákli, Imre	Przybylski, Michael	Oláh, Julianna	Linder, Mats L.
17:20 – 17:40	Wagner, István	Tömböly, Csaba	Gyurcsik, Béla	Hall, Melanie
17:40 – 18:00	Pálmai, Marcell	Uversky, Vladimir	Chatterjee, Sunanda	Otero, Toribio F.
14:00 – 17:00	Tutorials Towards Biology Tutorial 4: <i>How living cells work: structure and function</i> Instructor: Peter Lów (ELTE, Dept. Anatomy, Cell and Developmental Biology)			<i>(0.87 Marx Hall)</i>
18:00 – 19:00 Poster Session I (<i>Poster session area</i>)				
20:30 – Organ Concert at the Szt. Anna Church (Budapest, Batthány tér 7)				

Friday, 2 September 2011				
8:30 – 9:15	Wolfgang Lubitz		Plenary Lecture (-1.75 Conference Hall)	
Parallel sessions:				
	(0.89 Jedlik Hall)	(-1.75 Conference Hall)	(0.81 Ortway Hall)	(0.83 Eötvös Hall)
	BIO-NANOTECHNOLOGY	FRONTIERS IN MEDICINAL CHEMISTRY	BIOINORGANIC CHEMISTRY	SYNTHETIC BIOLOGY
9:20 – 9:50	Ghibaudi, Elena M.	Leeson, Paul	Horváth, Ottó	Mansy, Sheref
9:50 – 10:10	Mártonfalvi, Zsolt	Simon, Zoltán	Jancsó, Attila	Stano, Pasquale
10:10 – 10:30	Sztrik, Attila	Adamowicz, Agnieszka	Orlova, Sofiya	Antonczak, Alicja K.
10:30 – 10:50	Wagner, Zsolt	Breytenbach, Jaco	Várnagy, Katalin	Pósfai, György
10:50 – 11:10	Khoramnejadian, Shahrzad	Mándity, István	Hémadi, Miryana	Papp, Balázs
11:10 – 11:30	Coffee Break (Ground floor, next to the Spherical Hall)			
Parallel sessions:				
	(0.89 Jedlik Hall)	(-1.75 Conference Hall)	(0.81 Ortway Hall)	(0.83 Eötvös Hall)
	NUCLEIC ACIDS	FRONTIERS IN MEDICINAL CHEMISTRY	NEUROCHEMISTRY AND NEURODEGENERATION	METALS IN MEDICINE
11:30 – 11:50	Vértessy, Beáta	Ye, Tao	Fülöp, Livia	Di Marco, Valerio
11:50 – 12:10	Engels, Joachim W.	Varga, Gergely	Salifoglou, Thanos	Hadjikakou, Sotiris
12:10 – 12:30	Horváth, András	Kohei, Imai	Juhász, Gábor	Enyedi, Éva
12:30 – 12:50	Linkorn, Soeren	–	Grimm, Marcus	–
10:00 – 13:00	Tutorials Towards Biology Tutorial 8: 21st-century Enzymology Instructor: Mihály Kovács (ELTE, Dept. Biochemistry)			(0.87 Marx Hall)
12:30 – 13:30	Poster Section II (Poster session area)			
12:30 – 14:30	Lunch (First floor, adjacent to the Spherical Hall)			
14:30–	Excursion to Visegrád and Banquet on the Hunyadi Boat on the River Danube			
Saturday, 3 September 2011				
Parallel sessions:				
	(0.89 Jedlik Hall)	(-1.75 Conference Hall)	(0.81 Ortway Hall)	(0.83 Eötvös Hall)
	NUCLEIC ACIDS	FRONTIERS IN MEDICINAL CHEMISTRY	ARTIFICIAL PHOTOSYNTHESIS	METALS IN MEDICINE
8:30 – 9:00	Nordén, Bengt	Giralt, Ernest	de Groot, Huub	Alberto, Roger
9:00 – 9:20	Tedeschi, Tullia	Boyapati, Shireesha	Murray, James	Jakusch, Tamás
9:20 – 9:40	Klimasauskas, Saulius	Caballero, Esther	Yang, Chunhong	Tomaz, Ana Isabel
9:40 – 10:00	Guga, Piotr	Fukuda, Takeshi	Garab, Győző	Fakhre, Nabil A.
10:00 – 10:20	Reymer, Anna	–	Valicsek, Zsolt	–
10:20 – 10:40	Coffee Break (Ground floor, adjacent to the Spherical Hall)			
Parallel sessions:				
	(0.89 Jedlik Hall)	(-1.75 Conference Hall)	(0.81 Ortway Hall)	
	NUCLEIC ACIDS	FRONTIERS IN MEDICINAL CHEMISTRY	BIOGEOCHEMISTRY	
10:40 – 11:00	Mueller, Sabine	Demizu, Yosuke	Kaestner, Matthias	
11:00 – 11:20	Várallyay, Éva	Elkaim, Judith	Tugarova, Anna V.	
11:20 – 11:40	Vellai, Tibor	Chang, Ta-Chau	Kadyshevich, Elena A.	
11:40 – 12:00	–	Zerbe, Oliver	Dykman, Roman L.	
12:00 – 12:45	Julio Fernandez		Plenary Lecture (-1.75 Conference Hall)	
12:45 – 13:15	Closing Ceremony		(-1.75 Conference Hall)	
	Poster Awards			
13.15 – 14.30	Lunch			

Wednesday, 31 August 2011

- 10:00 – 16:00 Registration
(Eötvös Loránd University, Budapest, Pázmány Péter sétány 1/A; Entrance from the river side)
- 13:00 – 16:00 **Tutorials Towards Biology**
Tutorial 2: *Macromolecular interactions* (0.87 Marx Hall)
Instructor: **József Kardos** (ELTE, Dept. Biochemistry)
- 16:00 – 17:00 Opening ceremony (-1.75 Conference Hall)
- 17:00 – 17:45 *Plenary Lecture* (-1.75 Conference Hall)
Chair: **Henryk Kozłowski** (University of Wrocław)
- Ivano Bertini**
METAL IONS IN AND FOR STRUCTURAL BIOLOGY
- 17:45 – 18:30 *Plenary Lecture* (-1.75 Conference Hall)
Chair: **András Perczel** (Eötvös University)
- Dieter Seebach**
 β -PEPTIDES - FROM ORGANIC SYNTHESIS TO BIOCHEMISTRY, BIOLOGY, MEDICINAL CHEMISTRY ... AND BACK
- 18:30 – 20:30 Get-together party (1st floor, adjacent to the Spherical Hall)

Thursday, 1 September 2011

- 9:00 – 9:45 *Plenary Lecture* (-1.75 Conference Hall)
Chair: **Tamás Gajda** (University of Szeged)
- Bernt Krebs**
COOPERATIVITY IN DINUCLEAR IRON AND COPPER ENZYMES: PURPLE ACID PHOSPHATASES AND CATECHOL OXIDASES
- PARALLEL SESSIONS**
- Peptide/protein Bioconjugates for Diagnosis and Therapy**
Chair: **Ferenc Hudecz**, Hungary (0.89 Jedlik Hall)
- 9:50 – 10:10 G. Sármay, E. Szarka, J. Pozsgay, D. Szili, F. Babos, Gy. Nagy, B. Rojkovich, A. Magyar, F. Hudecz
CITRULLIN CONTAINING PEPTIDES AS B-CELL EPITOPES
- 10:10 – 10:30 M. Taki, T. Hamamoto, M. Sisido
SYNTHESIS OF CYCLIC PEPTIDES/PROTEINS USING THE NEXT-A CYCLIZATION REACTION
- 10:30 – 10:50 Zbigniew Zawada, Martin Šafařík, Eva Dvořáková, Anna Březinová, Jaroslav Šebestík, Ivan Stibor, Karel Holada, and Petr Bouř
REACTIVITY OF 9-CHLOROACRIDINES TOWARD PEPTIDES THIOL GROUP: EXPERIMENTAL AND THEORETICAL STUDY
- 10:50 – 11:10 Yemi Datsmol, Balpreet Matharu, Nick Spencer and Brian Austen
SYNTHESIS OF GADOLINIUM-COMPLEXED BETA-AMYLOID-BINDING PEPTIDES AS CONTRAST AGENTS FOR MRI DIAGNOSIS OF ALZHEIMER'S DISEASE
- 11:10 – 11:30 **Coffee Break** (Ground floor, adjacent to the Spherical Hall)

11:30 – 12:00	<i>Keynote lecture</i> Charlotte A. E. Hauser A CLASS OF ULTRASMALL ALIPHATIC PEPTIDES SELF-ASSEMBLE TO AMYLOID-LIKE FIBROUS SCAFFOLDS: RATIONAL DESIGN OF NEW BIOMATERIALS AND THERAPEUTICS
12:00 – 12:20	<u>P. Boisguerin</u> , C. Redt-Clouet, A. Franck-Mielo, S. Barrère-Lemaire and B. Lebleu CPP DELIVERY OF APOPTOSIS-REGULATING PEPTIDES TO PREVENT REPERFUSION LESIONS IN MICE HEART
12:20 – 12:40	<u>K. Nokihara</u> , A. Hirata, T. Ohyama, T. Sogon, Y. Oka, Y. Takebayashi, R. Morisita, K. Kasai, <u>T. Yokoyama</u> and S. Mohri THE CONSTRUCTION OF A NOVEL BIODETECTION SYSTEM USING DESIGNED PEPTIDE DERIVATIVES ARRIVED ON A NOVEL PLATE MADE FROM AMORPHOUS CARBON
12:40 – 13:00	<u>S. Els</u> , C. Chollet, A.G. Beck-Sickinger DESIGN AND SYNTHESIS OF GHRELIN RECEPTOR INVERSE AGONISTS AN APPLICATION FOR OBESITY TREATMENT
<i>Dynamics in Biology: Structural Disorder, Molecular Dynamics, Folding, and Misfolding of Proteins</i>	
Chairs: Péter Tompa , Hungary and Robert Konrat , Austria (-1.75 Conference Hall)	
9:50 – 10:10	<u>G. Horváth</u> , G. Tárkányi, O. Tőke INTERNAL MOTIONS AND EXCHANGE PROCESSES IN HUMAN ILEAL BILE ACID-BINDING PROTEIN
10:10 – 10:30	<u>R. Arora</u> , S. Abdel-Azeim, M. Gottikh, L. Tchertanov THE DNA RECOGNITION BY THE HIV-1 INTEGRASE: COMPUTATIONAL STUDY OF THE WILD TYPE AND R228A MUTANT
10:30 – 10:50	<u>Pires RH</u> , Saraiva MJ, Damas AM, Kellermayer MS AMYLOID PROTEIN AGGREGATION: STRUCTURAL TRANSITIONS OBSERVED BY ATOMIC FORCE MICROSCOPY AND FORCE SPECTROSCOPY
10:50 – 11:10	<u>A. H. C. Horn</u> , H. Sticht A SYSTEMATIC MOLECULAR DYNAMICS STUDY OF AMYLOID- β 42 OLIGOMER STRUCTURES FROM FIBRILS
11:10 – 11:30	Coffee Break (Ground floor, adjacent to the Spherical Hall)
11:30 – 12:00	<u>Gábor Harami</u> , Máté Gyimesi, Kata Sarlós, Mihály Kovács ENZYMATIC PROCESSES IN DNA REPAIR
12:00 – 12:20	<u>Andrea Lakatos</u> , Yean Sin Ong, Klaas Martinus Pos and Clemens Glaubitz SOLID-STATE NMR STUDIES ON SUBSTRATE-EMRE INTERACTIONS
12:20 – 12:40	<u>G. Batta</u> , Á. Fizil, M. Nyitrai, V. Tomori, T. Barna, K. E. Kövér, G. Tóth, G. Váradi, Z. Kele, Á. Somogyi, Z. Gáspári, É. Leiter, I. Pócsi and F. Marx DISULFIDE BOND TOPOLOGY: SYNTHETIC AND MASS SPECTROSCOPY HURDLES
12:40 – 13:00	<u>P. Rovó</u> , A. Láng, P. Stráner, A. Perczel NMR CHARACTERIZATION OF THE INTERMEDIATE STATE OF TRP-CAGE MINIPROTEINS
<i>Computed Molecular Properties in Life Sciences, Computational Aspects of Biomolecules, Chemical Bioinformatics</i>	
Chairs: Gábor Náray-Szabó , Hungary and G. Matthias Ullmann , Germany (0.81 Ortvay Hall)	
9:50 – 10:10	<u>Snežana D. Zarić</u> NONCOVALENT INTERACTIONS OF AROMATIC RINGS IN PROTEINS
10:10 – 10:30	<u>Z. Marton</u> , M. Rhimi, P. Lallemand, L. P. Jordheim, C. Dumontet, N. Aghajari, C. Lionne, S. Peyrottes and <u>L. Chaloin</u> IN SILICO DESIGN OF NEW INHIBITORS AGAINST CYTOSOLIC 5'-NUCLEOTIDASE II

10:30 – 10:50	<u>S.A. Wieninger</u> , E.H. Serpersu, G.M. Ullmann DIFFERENTIAL EFFECTS OF ATP AND AMINOGLYCOSIDE BINDING ON PROTEIN DYNAMICS – A GAUSSIAN NETWORK ANALYSIS
10:50 – 11:10	C. Colas, F. Roussi, <u>B.I. Iorga</u> FOCUSED LIGAND LIBRARIES AS TOOLS FOR <i>IN SILICO</i> DESIGN OF ANTI-APOPTOTIC PROTEINS INHIBITORS
11:10 – 11:30	Coffee Break <i>(Ground floor, adjacent to the Spherical Hall)</i>
11:30 – 12:00	<i>Keynote lecture</i> <u>Zoltan Mucsi</u> , Péter Ábrányi-Balogh, Bela Viskolcz, Gregory A. Chass, <u>Imre G. Csizmadia</u> ENERGY MANAGEMENT AT THE MOLECULAR LEVEL IN THE LIVING CELL. A THEORETICAL ANALYSIS FROM A SYSTEM CHEMISTRY POINT OF VIEW
12:00 – 12:20	Andrea Bottoni, Matteo Calvaresi, <u>Gian Pietro Miscione</u> EXPLORING ENZYME MECHANISMS: A QM APPROACH
12:20 – 12:40	<u>Tamás Beke-Somfai</u> , Per Lincoln, Bengt Nordén A QUANTUM MECHANICAL STUDY ON THE REACTION MECHANISM IN ATP SYNTHASE
12:40 – 13:00	<u>D. Kozma</u> , I. Simon, G. E. Tusnády STRUCTURE PREDICTION OF ALPHA-HELICAL TRANSMEMBRANE PROTEINS
	<i>Glycochemistry - Glycoscience</i>
	Chairs: László Somsák , Hungary and Stefan Oscarsson , Ireland <i>(0.83 Eötvös Hall)</i>
9:50 – 10:10	<u>Gordon K. Gomba</u> , Manuel A. Coimbra, Jana Čopíková, Claudia Nunes, Andriy Synytsya SUGAR COMPOSITION AND LINKAGE ANALYSIS OF FUNGAL POLYSACCHARIDES
10:10 – 10:30	M.B. Thygesen, J. Sauer, N. N. Maolanon, K. K. Sørensen, J. Stougaard, <u>K. J. Jensen</u> NEW CHEMOSELECTIVE TOOLS FOR GLYCOCONJUGATES AND GLYCONANOSCIENCE
10:30 – 10:50	Evangelia D. Chrysina STRUCTURE-BASED INHIBITOR DESIGN OF GLYCOGEN PHOSPHORYLASE- AN INTERDISCIPLINARY APPROACH FOR THE TREATMENT OF TYPE 2 DIABETES
10:50 – 11:10	<u>M. Czugler</u> , I. Pintér SODIUM-SUGAR CO-TRANSPORT STRUCTURE MODELS
11:10 – 11:30	Coffee Break <i>(Ground floor, adjacent to the Spherical Hall)</i>
11:30 – 12:00	<i>Keynote lecture</i> O. Hindsgaul SYNTHETIC CHEMISTRY YIELDS NEW TOOLS FOR GLYCOBIOLOGY
12:00 – 12:20	<u>Y.-H. Tsai</u> , S. Götze, P. H. Seeberger, <u>D. Varón Silva</u> SYNTHESIS OF GLYCOSYLPHOSPHATIDYLINOSITOL-ANCHORED PRION PROTEIN
12:20 – 12:40	<u>A. Borbás</u> , M. Herczeg, L. Lázár, E. Mező, Zs. Bereczky; <u>A. Lipták</u> ; S. Antus SULFONIC ACID ANALOGUES OF THE ANTITHROMBIN-BINDING DOMAIN OF HEPARIN
12:40 – 13:00	P. Fügedi SUBSTITUENT, STEREOELECTRONIC AND SOLVENT EFFECTS IN GLYCOSYLATIONS
10:00 – 13:00	<i>Tutorials Towards Biology</i> Tutorial 3: <i>Essential gene technology for chemists</i> <i>(0.87 Marx Hall)</i> Instructor: László Nyitray (ELTE, Dept. Biochemistry)
13:00 – 14:50	Lunch <i>(First floor, adjacent to the Spherical Hall)</i>

PARALLEL SESSIONS***Peptide/protein Bioconjugates for Diagnosis and Therapy***Chair: **Ferenc Hudecz**, Hungary

(0.89 Jedlik Hall)

14:50 – 15:20

Keynote lecture

A. Bodor, A. Láng, A. Perczel, K. Kövér, P. Rapali, L. Radnai, L. Nyitray
 PROTEIN-PEPTIDE INTERACTION BETWEEN A DYNEIN LIGHT CHAIN AND
 AN UNSTRUCTURED MYOSIN FRAGMENT

15:20 – 15:40

G. Mező, A. Szabó, E. Lajkó, I. Szabó, M. Manea, O. Láng, L. Kóhidai
 PEPTIDE-DRUG BIOCONJUGATES CONTAINING DIFFERENT TARGETING MOIETIES

15:40 – 16:00

V.M. Ahrens, R. Frank, E. Hey-Hawkins, A.G. Beck-Sickinger
 SYNTHESIS AND INCORPORATION OF *ORTHO*- CARBAMBOXY-L- ϵ -MODIFIED
 L-LYSINE INTO PEPTIDES

16:00 – 16:20

J. Láng, K. Pomázi, Sz. Bösze, G. Mező, F. Hudecz, L. Kóhidai
 INFLUENCE OF PHYSICOCHEMICAL MOIETIES OF WSXWS-OLIGOTUFTSIN
 CONJUGATES ON ADHESION AND CHEMOTAXIS

16:20 – 16:40

R. Pipkorn, M. Wiessler, L. Dunsch, M. Bock, W. Waldeck, Klaus Braun
 FUNCTIONALIZATION OF AMIDE-MONOMERS WITH ENDOHEDRAL GD-N-CLUSTER-
 FULLERENE & SYNTHESIS OF BIOSHUTTLE CONJUGATES APPROPRIATE AS
 MR-CONTRAST AGENTS?

16:40 – 17:00

Coffee Break

(Ground floor, adjacent to the Spherical Hall)

Bio-nanotechnology: Visualization and Manipulation of Individual Bio-macromoleculesChairs: **Mikós Kellermayer**, Hungary and **Julio Fernandez**, United States

(0.89 Jedlik Hall)

17:00 – 17:20

Imre Jákl, Bertalan Kovács, András Perczel
 LOCAL CONFORMATIONAL STUDY OF BETA SHEET BUILDING UNITS

17:20 – 17:40

I. Wagner, Zs. K. Nagy, G. Drávavölgyi, A. H. Harasztos, Á. Suhajda, G. Marosi
 ELECTROSPUN BIOHYBRID NANOFIBERS FOR DRUG DELIVERY

17:40 – 18:00

Marcell Pálmai, Livia Naszályi Nagy, Judith Mihály, Tibor Kremmer
 PREPARATION, PURIFICATION AND CHARACTERIZATION OF AMINO-
 FUNCTIONALIZED SILICA SOL

Biomolecules in 3DChairs: **Zoltán Gáspári**, Hungary and **Janez Plavec**, Slovenia

(-1.75 Conference Hall)

14:50 – 15:20

Nicolas Wolff, Elouan Terrien, Nicolas Babault, Christophe Préhaud, Mireille Lafage,
 Matthias J. Schnell, Henri Buc, Monique Lafon, Florence Cordier and Muriel Delepierre
 MOLECULAR BASIS OF VIRAL PATHOGENICITY

15:20 – 15:40

D. Héja, A. Kocsis, J. Dobó, A. K. Kékesi, R. Szász, V. Harmat, P. Závodszy, P. Gál, G. Pál
 DIRECTED EVOLUTION OF PEPTIDE AND SMALL PROTEIN INHIBITORS OF KEY
 COMPLEMENT PROTEASES

15:40 – 16:00

P. Šket, P. Podbevšek, J. Plavec
 NMR STUDIES OF CATION INTERACTIONS WITH G-QUADRUPLEXES

16:00 – 16:20

P. Rapali, Á. Szenes, L. Radnai, A. Bakos, V. Grolmusz, G. Pál, L. Nyitray
 DYNLL/LC8: A HUB PROTEIN THAT RECOGNIZES LINEAR PEPTIDE MOTIFS
 LOCALIZED IN DISORDERED SEGMENTS OF ITS INTERACTION PARTNERS

16:20 – 16:40

Michael C. Owen, Milán Szóri, Imre G. Csizmadia and Béla Viskolcz
 RADICAL INITIATED UNFOLDING OF PEPTIDES AND PROTEINS

16:40 – 17:00

Coffee Break

(Ground floor, adjacent to the Spherical Hall)

Neurochemistry; Molecular Mechanism of NeurodegenerationChairs: **Botond Penke**, Hungary and **Michael Przybylski**, Germany (-1.75 Conference Hall)

- 17:00 – 17:20 Michael Przybylski
MASS SPECTROMETRIC APPROACHES FOR ELUCIDATION OF “MISFOLDING” AND AGGREGATION STRUCTURES OF NEURO-DEGENERATIVE PROTEINS: ION MOBILITY-MS AND AFFINITY-MS
- 17:20 – 17:40 B. Schäfer, M. Majer, E. Welker, Cs. Tömböly
PREPARATION OF PRION PROTEIN DERIVATIVES
- 17:40 – 18:00 Vladimir Uversky
INTRINSICALLY DISORDERED PROTEINS IN NEURODEGENERATIVE DISEASES

New Trends in Bioinorganic Chemistry: Metals and MetalloproteinsChairs: **Tamás Gajda**, Hungary and **Henryk Kozłowski**, Poland (0.81 Ortway Hall)

- 14:50 – 15:20 *Keynote lecture*
Henryk Kozłowski, Karolina Krzywoszynska, Sławomir Potocki, Magdalena Rowinska-Zyrek, Daniela Valensin and Danuta Witkowska
SPECIFIC METAL ION BINDING TO HISTIDINE-RICH AND CYSTEINE-RICH REGIONS IN PROTEINS
- 15:20 – 15:40 D. Árus, Á. Dancs, T. Gajda, N.V. Nagy
A COMPARATIVE STUDY ON THE POSSIBLE METAL-BINDING SITES OF THE HUMAN ZnT3 ZINC-TRANSPORTER PROTEIN
- 15:40 – 16:00 NT. Ha-Duong, C. Eid, M. Hémedi, JM. El Hage Chahine
MECHANISM OF IRON UPTAKE BY CERULOPLASMIN
- 16:00 – 16:20 M. Rowinska-Zyrek, D. Witkowska, D. Valensin and H. Kozłowski
BISMUTH DISPLACES NICKEL FROM IT'S BINDING SITES IN CYSTEINE RICH SEQUENCES
- 16:20 – 16:40 E. Gumienna-Kontecka, I.O. Fritsky
BIOLOGICALLY RELEVANT SPECIFIC METAL COORDINATION BY HYDROXAMIC ACIDS AND OXIMES
- 16:40 – 17:00 **Coffee Break** (Ground floor, adjacent to the Spherical Hall)
- 17:00 – 17:20 J. Oláh
QM AND QM/MM MODELLING OF DRUG METABOLISM BY CYTOCHROME P450 ENZYMES
- 17:20 – 17:40 B. Gyurcsik, A. Czene, N.I. Simon, E. Németh, I.G. Zóka, T. Körtvélyesi, H.E.M. Christensen, K. Nagata
STUDY ON THE HNH MOTIF AS A POSSIBLE COMPONENT OF A CONTROLLED ZINC-FINGER NUCLEASE
- 17:40 – 18:00 S. Chatterjee, E. Galardon, M.A. Sari and I. Artaud
COMPLEXATION AND OXIDATION OF SYNTHETIC REDUCED CYCLIC MOUSE HEPCIDINE ANALOG WITH FE(III)

From Bioinspired Organocatalysis to Enzyme Catalysis: Mechanisms and Functions, Molecular Recognition and BiocatalysisChair: **Tibor Soós**, Hungary (0.83 Eötvös Hall)

- 14:50 – 15:20 *Keynote lecture*
D. Enders
ASYMMETRIC ORGANOCATALYSIS: METHODS AND APPLICATIONS
- 15:20 – 15:40 Frank Jordan
OBSERVATION OF INTERMEDIATES ON THIAMIN ENZYMES PYRUVATE & 2-OXOGLUTARATE MULTIENZYME COMPLEXES

15:40 – 16:00	Gábor Tárkányi SELF-ASSOCIATION OF AMINE-THIOUREA ORGANOCATALYSTS	
16:00 – 16:20	Andrei Ursu, Ashish Tiwari, Franz P. Schmidtchen ENTROPY IN MOLECULAR RECOGNITION: PROBING THE ROLE OF SOLVENT IN ION PAIRING AND CHIRAL DISCRIMINATION	
16:20 – 16:40	P. Lallemand, L. Chaloin, B. Roy, T. Barman, M. W. Bowler, C. Lionne INTERACTION OF HUMAN 3-PHOSPHOGLYCERATE KINASE WITH THE TWO ENANTIOMERS OF ADP	
16:40 – 17:00	Coffee Break	<i>(Ground floor, adjacent to the Spherical Hall)</i>
17:00 – 17:20	Mats Linder, Tore Brinck COMPUTATIONAL ENGINEERING OF ENZYMES: STRATEGIES FOR DESIGNING DIELS-ALDERASES	
17:20 – 17:40	M. Hall, C. K. Winkler, C. Stueckler, K. Zangger, K. Faber ENZYMATIC SYNTHESIS OF ENANTIOPURE α,β -AMINO ACID DERIVATIVES USING FLAVOPROTEINS FROM THE 'OLD YELLOW ENZYME' FAMILY	
17:40 – 18:00	T.F. Otero, J. Arias-Pardilla, J.G. Martínez, P. Giménez and Y. Ismail DENSE, REACTIVE, IONIC AND WET GELS AS BIOMIMICKING MODEL REACTIONS AND BIOMIMICKING DEVICES	
14:00 – 17:00	Tutorials Towards Biology Tutorial 4: <i>How living cells work: structure and function</i> Instructor: Peter Lów (ELTE, Dept. Anatomy, Cell and Developmental Biology)	<i>(0.87 Marx Hall)</i>
18:00 – 19:00	Poster Session I	<i>(Poster session area)</i>
20:30 –	<i>Organ Concert at the Szt. Anna Church (Budapest, Batthány tér 7)</i>	

Friday, 2 September 2011

8:30 – 9:15	<i>Plenary Lecture</i> Chair: Győző Garab (Biological Research Center) Wolfgang Lubitz BIOLOGICAL CATALYSTS INVOLVED IN BIOSOLAR WATER SPLITTING AND HYDROGEN PRODUCTION	<i>(-1.75 Conference Hall)</i>
PARALLEL SESSIONS		
Bio-nanotechnology: Visualization and Manipulation of Individual Bio-macromolecules		
Chairs: Mikós Kellermayer , Hungary and Julio Fernandez , United States <i>(0.89 Jedlik Hall)</i>		
9:20 – 9:50	E. Ghibaudi, B. Boscolo, F. Turci, M. Colonna, I. Fenoglio, B. Fubini SDSL-EPR AS A TOOL FOR GRASPING TOPOLOGICAL INFORMATION ON THE INTERACTION BETWEEN PROTEINS AND NANOPARTICLES	
9:50 – 10:10	Zsolt Mártonfalvi, Pasquale Bianco, Miklós Kellermayer NANOMECHANICAL MANIPULATION OF SKELETAL-MUSCLE TITIN WITH FORCE-CLAMP OPTICAL TWEEZERS	
10:10 – 10:30	Attila Sztrik, Péter Eszenyi, Beáta Babka, József Prokisch FATE OF NANO SIZE SELENIUM IN BIOLOGICAL SYSTEMS	
10:30 – 10:50	Zsolt Wagner, Gábor Rácz, Erzsébet Bori, Tamás Tábi, Éva Szökő USING AMINO FUNCTIONALIZED ORMOSIL NANOPARTICLES AS A NON-VIRAL DNA VECTOR	
10:50 – 11:10	S. Khoramnejadian, J. Jamali Zavareh BIODEGRADABILITY OF POLYPROPYLENE BLEND	
11:10 – 11:30	Coffee Break	<i>(Ground floor, next to the Spherical Hall)</i>

Structural and Functional Diversity of Nucleic AcidsChairs: **Tibor Vellai**, Hungary and **Bengt Nordén**, Sweden

(0.89 Jedlik Hall)

11:30 – 11:50 Villő Muha, András Horváth, Angéla Békési, Imre Zagyva, Miklós Erdélyi, János Szabad, Beáta G. Vértessy
MULTIPLE ROLES OF URACIL IN DNA

11:50 – 12:10 J. W. Engels, O. Romainczyk, I. Krstić, T. F. Prisner, R. Hänsel, V. Dötsch
SYNTHESIS OF NITROXYL-SPIN-LABELED DNA/RNA AND DISTANCE MEASUREMENTS BY EPR-PELDOR/DEER

12:10 – 12:30 András Horváth, Villő Muha, Beáta G. Vértessy
QUANTITATIVE DETERMINATION OF DEOXYURIDINE IN DNA WITH THE HELP OF ARCHEAL DNA POLYMERASES

12:30 – 12:50 S. Linkorn, R. Stoltenburg, B. Strehlitz
DNA APTAMERS AS MOLECULAR RECOGNITION ELEMENTS FOR THE RAPID DETECTION OF PATHOGENS

Frontiers in Medicinal Chemistry, New Methods in Drug DesignChairs: **György Keserű**, Hungary and **Knud J. Jensen**, Denmark

(-1.75 Conference Hall)

9:20 – 9:50 *Keynote lecture*
Paul Leeson

ORGANISATIONAL VARIABILITY IN DRUG DESIGN: AN ASSESSMENT OF TARGET-UNBIASED COMPOUND QUALITY

9:50 – 10:10 Z. Simon, Á. Peragovics, M. Vigh-Smeller, G. Csukly, L. Tombor, Z. Yang, G. Zahoránszky-Kőhalmi, L. Végner, B. Jelinek, P. Hári, Z. Brandhuber, B. Bíró, D. Nagy, M. Marót, Cs. Hetényi, I. Bitter, P. Czobor, A. Málnási-Csizmadia
DRUG EFFECT PREDICTION BY *IN SILICO* GENERATED PROTEIN-SMALL MOLECULE AFFINITY PROFILES

10:10 – 10:30 A.L.Adamowicz, J.M.Dąbrowski, A.V.Simoes, M.M.Pereira, L.G.Arnaut, G. Stochel
PHYSICOCHEMICAL PROPERTIES OF NOVEL FLUORINATED SENSITIZERS FOR PHOTODYNAMIC THERAPY

10:30 – 10:50 Jaco C. Breytenbach, Marli C. Lombard, David D. N'Da, Carmen A. Lategan, Peter J. Smit & Henri Vial
SYNTHESIS AND BIOLOGICAL EVALUATION OF NEW ARTEMISININ HYBRIDS AS ANTIMALARIAL AGENTS

10:50 – 11:10 I. M. Mándity, P. Vainiotalo, F. Fülöp, J. Jänis
Probing secondary structure of β -PEPTIDE FOLDAMERS USING GAS-PHASE H/D EXCHANGE REACTIONS

11:10 – 11:30 **Coffee Break**

(Ground floor, next to the Spherical Hall)

11:30 – 11:50 Shoubin Tang, Zhuo Wang, Yuqing Liu, Xiaomin Zhang, Zhengshuang Xu, Tao Ye
DESIGN, SYNTHESIS AND BIOLOGICAL EVALUATION OF PCNA INHIBITORS TO BLOCK p53 PROTEOLYSIS

11:50 – 12:10 Gergely Varga, Andrea Sztankovics, János József, László Juhász, Tibor Docsa, Pál Gergely, László Somsák
SYNTHESIS OF ANALOGUES OF FR258900

12:10 – 12:30 Kohei Imai, Ikuo Nakanishi, Satomi Nakanishi, Ryohei Takagaki, Ken-ichiro Matsumoto, Kazunori Anzai, Toshihiko Ozawa, Haruhiro Okuda, Asao Nakamura Kiyoshi Fukuhara
SYNTHESIS OF CATECHIN DERIVATIVE WITH BASIC AMINO ACID AS A PROMISING ANTIOXIDANT

New Trends in Bioinorganic Chemistry: Metals and MetalloproteinsChairs: **Tamás Gajda**, Hungary and **Henryk Kozłowski**, Poland (0.81 Ortway Hall)

- 9:20 – 9:50 O. Horváth, Z. Valicsek, G. Harrach, G. Lendvay, M. A. Fodor
PHOTOPHYSICAL AND PHOTOCHEMICAL PROPERTIES OF WATER-SOLUBLE METALLOPORPHYRINS: THE ROLE OF THE DISTORTED STRUCTURE
- 9:50 – 10:10 A. Jancsó, B. Gyurcsik, D. Szunyogh, A. Angyal, L. Szekeres, L. Hemmingsen, F.H. Larsen, P.W. Thulstrup, N.J. Christensen
EQUILIBRIUM AND SOLUTION STRUCTURAL STUDIES ON THE INTERACTION OF CADMIUM(II) AND MERCURY(II) WITH CYSTEINE CONTAINING OLIGOPEPTIDES
- 10:10 – 10:30 S.I. Orlova, N.N. Meleshonkova, E.R. Milaeva, E.F. Shevtsova
THE ANTIOXIDATIVE ACTIVITY MECHANISM OF 2,6-DI-TERT-BUTYLPHENOL CONTAINING FERROCENES
- 10:30 – 10:50 K. Várnagy
COORDINATION ABILITY OF AMINO ACID AND PEPTIDE DERIVATIVES CONTAINING VARIOUS DONOR ATOMS
- 10:50 – 11:10 M. Hémadi, NT. Ha-Duong and JM. El Hage Chahine
MECHANISM OF THE URANYL-TRANSFERRIN COMPLEX FORMATION
- 11:10 – 11:30 **Coffee Break** (Ground floor, next to the Spherical Hall)

Neurochemistry; Molecular Mechanism of NeurodegenerationChairs: **Botond Penke**, Hungary and **Michael Przybylsky**, Germany (0.81 Ortway Hall)

- 11:30 – 11:50 L. Fülöp, D. Simon, Z. Bozsó, T. Janáky, M. Deli, A. Tóth, S. Veszelka, B. Penke
PROBLEMS OF CONTROLLING THE AGGREGATION OF THE SYNTHETIC BETA AMYLOID PEPTIDE FOR USE IN BIOLOGICAL EXPERIMENTS
- 11:50 – 12:10 A. Salifoglou
THE INTERACTION CHEMISTRY OF BIOTOXIC ALUMINUM WITH HYDROXYCARBOXYLIC ACIDS IN AQUEOUS MEDIA
- 12:10 – 12:30 A. Czurkó, G. Juhász, Zs Kovács, P. Baracska, P. Gulyácssy, T. Bártfai, KA.Kékesi
FROM PHYSIOLOGY TO PROTEOME: INFLAMMATION AND EPILEPSY HAS COMMON MOLECULAR MECHANISMS
- 12:30 – 12:50 Marcus Grimm
FROM BRAIN TO FOOD: MECHANISTICAL APPROACHES TO DETERMINE THE INFLUENCE OF FATTY ACIDS IN ALZHEIMER'S DISEASE

Synthetic Biology: from Molecules to Synthetic CellsChairs: **György Pósfai**, Hungary and **Sven Panke**, Switzerland (0.83 Eötvös Hall)

- 9:20 – 9:50 *Keynote lecture*
Sheref S. Mansy
RNA CONTROLLED CELL-LIKE SYSTEMS
- 9:50 – 10:10 Pasquale Stano, Pier Luigi Luisi
TOWARDS THE CONSTRUCTION OF SEMI-SYNTHETIC MINIMAL CELLS
- 10:10 – 10:30 Alicja K. Antonczak, Zuzana Simova and Dr. Eric Tippmann
GENETICALLY ENCODED NONNATURAL AMINO ACIDS: NOVEL METHODS FOR BIOENGINEERING STRUCTURE AND FUNCTION OF PROTEINS
- 10:30 – 10:50 György Pósfai
EVOLUTIONARY POTENTIAL OF ESCHERICHIA COLI CELLS WITH RE-DESIGNED GENOMES
- 10:50 – 11:10 Balázs Szappanos, Károly Kovács, Béla Szamecz, Frantisek Honti, Michael Costanzo, Anastasia Baryshnikova, Gabriel Gelius-Dietrich, Martin J. Lercher, Márk Jelasity, Chad L. Myers, Brenda J. Andrews, Charles Boone, Stephen G. Oliver, Csaba Pál, Balázs Papp
SYSTEMS BIOLOGY OF GENETIC INTERACTIONS IN YEAST METABOLISM
- 11:10 – 11:30 **Coffee Break** (Ground floor, next to the Spherical Hall)

Metals in MedicineChairs: **Imre Sóvágó**, Hungary and **Sotiris Hadjikakou**, Greece (0.83 Eötvös Hall)

11:30 – 11:50 A. Dean, É. Zsigó, É. Sija, M.G. Ferlin, D. Badocco, P. Pastore, A. Venzo, R. Bertani, T. Kiss, V.B. Di Marco
CHEMICAL EVALUATION OF HYDROXYPYRIDINECARBOXYLIC ACIDS AS NEW POSSIBLE CHELATING AGENTS FOR IRON AND ALUMINIUM

11:50 – 12:10 Sotiris K. Hadjikakou, Nick Hadjiliadis
THE USE OF ORGANOTIN, GOLD, ANTIMONY AND SILVER COMPOUNDS AS POTENTIAL CANCER METALLOTHERAPEUTICS

12:10 – 12:30 É.A. Enyedy, C.R. Kowol, É. Zsigó, T. Jakusch, N.V. Nagy, M.F. Primik, V.B. Arion, B.K. Keppler, T. Kiss
INTERACTION OF TRIAPINE AND RELATED THIOSEMICARBAZONES WITH VARIOUS METAL IONS: COMPARATIVE SOLUTION EQUILIBRIUM STUDIES

Tutorials Towards BiologyTutorial 8: *21st-century Enzymology*

(0.87 Marx Hall)

Instructor: **Mihály Kovács** (ELTE, Dept. Biochemistry)12:30 – 13:30 **Poster Session II**

(Poster session area)

12:30 – 14:30 **Lunch**

(First floor, adjacent to the Spherical Hall)

14:30 – *Excursion to Visegrád and Banquet on the Hunyadi Boat on the River Danube***Saturday, 3 September 2011****PARALLEL SESSIONS****Structural and Functional Diversity of Nucleic Acids**Chairs: **Tibor Vellai**, Hungary and **Bengt Nordén**, Sweden

(0.89 Jedlik Hall)

8:30 – 9:00 *Keynote lecture*

Bengt Nordén

POLARIZED LIGHT SPECTROSCOPY ON DNA, PROTEINS AND MEMBRANES

9:00 – 9:20 T. Tedeschi, A. Tonelli, S. Sforza, R. Corradini and R. Marchelli

DESIGN AND SYNTHESIS OF NEW FLUORESCENT PNAS FOR HIGH SPECIFIC NUCLEIC ACIDS RECOGNITION

9:20 – 9:40 Z. Liutkevičiūtė, E. Kriukienė, G. Lukinavičius, V. Masevičius, T. Khare, S.C. Wang, A. Petronis, S. Klimašauskas

EXCHANGE AND DERIVATIZATION OF 5-HYDROXYMETHYL GROUPS CATALYZED BY CYTOSINE METHYLTRANSFERASES

9:40 – 10:00 P. Guga, M. Janicka, A. Maciaszek, B. Rębowska, A. Tomaszewska, M. Dziedzic

HOOGSTEEN PAIRED HOMOPURINE [ALL-R_p-PS]-DNA OLIGOMERS AND HOMOPYRIMIDINE RNA, 2'-OMe-RNA OR 2'-OMe-RNA/LNA STRANDS FORM THERMALLY STABLE PARALLEL DUPLEXES

10:00 – 10:20 Anna Reymer, Karolin Frykholm, Per Lincoln and Bengt Nordén

A NEW LOOK AT DNA INTERCALATION

10:20 – 10:40 **Coffee Break**

(Ground floor, adjacent to the Spherical Hall)

10:40 – 11:00 S. Müller, B. Appel, D. Galla, H. Nguyen, N. Rublack, D. Springstube

SYNTHESIS OF FUNCTIONALIZED RNA: ESSENTIAL TOOLS FOR THE STUDY OF RNA STRUCTURE AND RIBOZYME FUNCTION

11:00 – 11:20 Éva Várallyay and Zoltán Havelda

VIRUSES CONTROL PLANT DEFENCE REACTION BY INTERFERING WITH SMALL REGULATORY RNA SYSTEM

11:20 – 11:40 Tibor Vellai

HOW DOES CHROMATIN STRUCTURE INFLUENCE SEXUAL DIFFERENTIATION?

Frontiers in Medicinal Chemistry, New Methods in Drug DesignChairs: **György Keserű**, Hungary and **Knud J. Jensen**, Denmark (-1.75 Conference Hall)

- 8:30 – 9:00 *Keynote lecture*
E. Giralt
NEW CHALLENGES IN STUDYING LIGAND-PROTEIN INTERACTIONS
- 9:00 – 9:20 Umasankar Kulathaivelu, Shireesha Boyapati, Venkatesan Jayaprakash, Raghuram Rao Akkinepally
SYNTHESIS AND ANTIVIRAL EVALUATION OF NOVEL DIHYDROPYRIMIDINES
- 9:20 – 9:40 E. Caballero, C. Pérez-Melero, M. De Sio, L. Aramburu, R. Álvarez, R. Peláez, M. Medarde
SYNTHESIS OF NOVEL POLYNITROGENATED DRUGS BASED ON PHENSTATINS
- 9:40 – 10:00 Takeshi Fukuda, Takeshi Kuribayashi, Yasuhiro Nakagami, Kazuki Yonekubo, Yumi Kawase
A NOVEL CC CHEMOKINE RECEPTOR 4 ANTAGONIST, SYNTHESIS AND STRUCTURE-ACTIVITY RELATIONSHIPS OF PYRIMIDINE DERIVATIVES
- 10:20 – 10:40 **Coffee Break** (Ground floor, adjacent to the Spherical Hall)
- 10:40 – 11:00 Yosuke Demizu, Yukiko Sato, Kyohei Horie, Ken-ichiro Takagi, Shinji Kakuda, Midori Takimoto-Kamimura, Haruhiro Okuda, Masaaki Kurihara
DESIGN OF NON-SECOSTEROIDAL VDR LIGANDS AND BINDING MODE TO VDR-LBD
- 11:00 – 11:20 J. Elkaïm, D. Bennani, M. Laguerre, J. Dessolin
FIRST IDENTIFICATION OF INHIBITORS OF PONTIN THROUGH VIRTUAL SCREENING
- 11:20 – 11:40 Ta-Chau Chang, Cheng-Chung Chang, Chi-Chih Kang, Zi-Fu Wang, Chih-Chien Cho
FROM FLUORESCENCE PROBES IN CANCER DIAGNOSIS TO G-QUADRUPLEX STABILIZERS FOR CANCER TREATMENT
- 11:40 – 12:00 S.L. Pedersen, V.K. Bhatia, S. Jurt, O. Zerbe, B. Holst, D. Stamou, N. Vrang, K. J. Jensen
DO PEPTIDE HORMONES BIND TO MEMBRANES PRIOR TO ACTIVATING THE RECEPTOR?

Artificial PhotosynthesisChairs: **Győző Garab**, Hungary and **Huub de Groot**, Netherland (0.81 Ortvay Hall)

- 8:30 – 9:00 S. Ganapathy, G.T. Oostergetel, M. Reus, A.G.M. Chew, F. Buda, E.J. Boekema, D.A. Bryant, S. Sengupta, P.K. Wawrzyniak, V. Huber, U. Baumeister, F. Würthner, A.R. Holzwarth, H.J.M. de Groot
ALTERNATING SYN-ANTI BACTERIOCHLOROPHYLLS FORM CONCENTRIC HELICAL NANOTUBES IN CHLOROSOMES AND FORM THE BASIS FOR SUPRAMOLECULAR LIGHT HARVESTING DYES
- 9:00 – 9:20 J.W. Murray
PROTEIN DESIGN FOR ARTIFICIAL PHOTOSYNTHESIS
- 9:20 – 9:40 Lei Zhang, Cheng Liu, Chunhong Yang
THE STRUCTURAL BASIS FOR REGULATING MACRO-ORGANIZATION STRUCTURE OF LIGHT HARVESTING CHLOROPHYLLA/B COMPLEXES OF PHOTOSYSTEM II (LHCIIb)
- 9:40 – 10:00 G. Steinbach, A. Zupcanova, M. Szabó, T. Jávorfí, S. Balaban, G. Garab
ANISOTROPIC ORGANIZATION 'ARTIFICIAL CHLOROSOMES', SELF-ASSEMBLED MICROMETER-SIZED RODS OF SYNTHETIC PORPHYRINS
- 10:00 – 10:20 Zsolt Valicsek and Ottó Horváth
POSSIBLE APPLICATION OF POST-TRANSITION AND LANTHANIDE METALLOPORPHYRINS IN ARTIFICIAL PHOTOSYNTHESIS
- 10:20 – 10:40 **Coffee Break** (Ground floor, adjacent to the Spherical Hall)

Microbes make the World go round. Biogeochemistry at Global Scale and DailyChairs: **Károly Márialigeti**, Hungary and **Matthias Kästner**, Germany (0.81 Ortway Hall)

- 10:40 – 11:00 M. Kästner
MICROBIAL DEGRADATION OF ORGANIC COMPOUNDS (NATURAL COMPOUNDS, XENOBIOTICS, AND PESTICIDES) AND THE FORMATION OF SOIL ORGANIC MATTER AND BIOGENIC NON-EXTRACTABLE RESIDUES
- 11:00 – 11:20 A.V. Tugarova, A.A. Kamnev, P.A. Tarantilis, M.G. Polissiou
IN SITU FTIR SPECTROSCOPIC ANALYSIS OF BACTERIAL INTRACELLULAR BIOMACROMOLECULES
- 11:20 – 11:40 E.A. Kadyshevich¹, V.E. Ostrovskii
GEOCHEMICAL PROCESSES AS THE BASIS FOR ORIGINATION OF THE EARTH BIOTA: FURTHER DEVELOPMENT OF THE LIFE ORIGINATION HYDRATE HYPOTHESIS (LOH-HYPOTHESIS)
- 11:40 – 12:00 A.A. Kamnev, R.L. Dykman, K. Kovács, A.V. Tugarova, E. Kuzmann, A. Vértes
SPECTROSCOPIC APPROACHES IN STUDYING MUTUAL EFFECTS OF SOIL IRON(III) AND MICROBIAL MOLECULAR SIGNALS

Metals in MedicineChairs: **Imre Sóvágó**, Hungary and **Sotiris Hadjikakou**, Greece (0.83 Eötvös Hall)

- 8:30 – 9:00 *Keynote lecture*
R. Alberto, D. Can, S. Sulieman, H. Braband, S. Imstepf, B. Spingler
TARGETING CYCLOPENTADIENYL COMPLEXES OF TECHNETIUM AND RHENIUM
- 9:00 – 9:20 T. Jakusch, É. Sija, É.A. Enyedy, C.G. Hartinger, B.K. Keppler, T. Kiss
SOLUTION EQUILIBRIUM STUDIES OF TERNARY COMPLEXES FORMED BETWEEN BIDENTATE (O,O;O,N;O,S) LIGANDS AND Ru^{III}EDTA OR Ru^{II}(η^6 -*p*-CYMENE)
- 9:20 – 9:40 A.I. Tomaz, T. Jakusch, T. S. Morais, R. F. M. de Almeida, F. Marques, F. Mendes, E. A. Enyedy, J. Costa Pessoa, T. Kiss, M. H. Garcia
[RU^{II}(H⁵-CP)(BPY)(PPH₃)]⁺, A PROMISING ANTITUMOR AGENT: AN *IN VITRO* STUDY REGARDING ITS BIOLOGICAL ACTIVITY
- 9:40 – 10:00 N. A. Fakhre and D. K. Ali
DETERMINATION OF IRON (II), IRON (III) AND TOTAL IRON IN SOME β -THALASSEMIA PATIENTS USING DIFFERENT ANALYTICAL TECHNIQUES
- 10:20 – 10:40 **Coffee Break** (Ground floor, adjacent to the Spherical Hall)

- 12:00 – 12:45 *Plenary Lecture* (-1.75 Conference Hall)
Chair: **Miklós Kellermayer** (Semmelweis University)
Julio M. Fernandez
FORCE-CLAMP SPECTROSCOPY OF SINGLE PROTEINS

- 12:45 – 13:15 **Closing Ceremony** (-1.75 Conference Hall)
Poster Awards

- 13.15 – 14.30 **Lunch**

POSTER PRESENTATIONS

Artificial Photosynthesis

- P1** L. Adrian, S.Szufa
BIOMASS TORREFACTION, THERMO-CHEMICAL DEGRADATION PROCESS FOR PRODUCTION OF GREEN BIO-FUELS

Biomolecules in 3D

- P2** Eunha Hwang, Hae-Kap Cheong, Chaejoon Cheong
CRYSTAL STRUCTURE OF SARAH DOMAIN FROM MST2 KINASE
- P3** Annamária F. Ángyán, Pál Stráner, Petra Rovó, András Perczel, Zoltán Gáspári
IN THE SEARCH OF PROTEIN STRUCTURAL CLASS SWITCHES
- P4** M. Kaliňák, J. Škorík, T. Liptaj, E. Varečka
FUNGAL GERMINATION, GROWTH AND CONIDIATION BY ¹H AND ¹³C NMR
- P5** M. A. McDowell, S. Johnson, J. E. Deane, D. M. Sheppard, M. Cheung, A. D. Roehrich, A. J. Blocker, J. M. McDonnell and S. M. Lea
THE SOLUTION STRUCTURE OF THE N-TERMINAL DOMAIN OF MXIG – A NEW MODEL SYSTEM FOR NMR?
- P6** D. Héja, K. Zboray, D. Szakács, A. Szabó, M. Sahin-Tóth and G. Pál
SELECTIVE INHIBITORS OF CHYMOTRYPSIN-C DEVELOPED BY PHAGE DISPLAY
- P7** Einat Schnur, Tali Scherf, Fred Naider and Jacob Anglister
THE CONFORMATION AND ORIENTATION OF A 27-RESIDUE CCR5 PEPTIDE IN A TERNARY COMPLEX WITH HIV-1 GP120 AND A CD4-MIMIC PEPTIDE
- P8** D. Szakács, E. Boros, D. Héja and G. Pál
THE OPTIMAL SERINE PROTEASE-INHIBITOR LOOP SEQUENCE IS SCAFFOLD DEPENDENT
- P9** Petros V. Gkazonis, Dionysios Vourtsis, Georgios A. Dalkas, Christos T. Chasapis, D. Bentrop, G.A. Spyroulias
A SOLUTION NMR STUDY OF NATIVE AND MUTATED FORMS OF THE ANTHRAX LETHAL FACTOR CATALYTIC SITE POLYPEPTIDE

Bio-nanotechnology: Visualization and Manipulation of Individual Bio-macromolecules

- P10** Youngseon Choi, Jeonghan Lee, Kumhyeon Kim, Heeyeon Kim, Peter Sommer and Rita Song
SYNTHESIS OF FRET-QUENCHED QUANTUM DOT-PEPTIDE PROBE FOR HIV-1 PROTEASE ACTIVITY IN VITRO AND IN VIVO
- P11** Balázs Kiss, Pál Röhlich and Miklós S.Z. Kellermayer
EFFECT OF DIVALENT CATION CHELATORS ON DESMIN DISASSEMBLY

Computed Molecular Properties in Life Sciences, Computational Aspects of Biomolecules, Chemical Bioinformatics

- P12** D.Zs. Badáczy, K. E. Németh, R. Kocsis, Zs.I. Németh
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- P13** J. Danis, T. Turányi
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- P14** Marcus Ennis, Zara Josephs, Gareth Owen, Björn Peters, Steve Turner, Randi Vita and Christoph Steinbeck
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- P15** Dávid Fazekas, Mihály Koltai, Zoltán Dúl, János Borda, Máté Pálffy, Dezső Módos, Máté Szalay-Bekő, Tibor Vellai, Péter Csermely, Illés J. Farkas, Tamás Korcsmáros
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- P16** B. Fiser, M. Szőri, B. Jójárt, R. Izsák, B. Viskolcz and I. G. Csizmadia
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- P17** G.V. Janjić, D.Ž Veljković, S.D. Zarić
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- P18** Gy. Juhász, O. Kysel, P. Mach
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- P19** B. Leitgeb
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- P20** M. Maruniak, E. Sedlárová, J. Csöllei, P. Mokry, I. Kapustíková
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- P22** G. Paragi, A. Bokros, J. Szolomajer, C. Fonseca Guerra, F. M. Bickelhaupt, L. Kovács
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- P23** Pică Elena Maria, Popișter Ioana, Bolunduț Liviu Călin, Neamțu Corina Ioana, Pirău Luminița Cristina, Duca Voicu
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- P25** D.V. Veres, Zs. Hoksza, E. Hazai, P. Csermely
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- P29** V. Farkas, P. Rovó, E. Vass, M. Hollósi, G. Tóth, A. Perczel
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