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The European Federation for Medicinal Chemistry (EFMC) is an independent association founded in 1970. Free from any political convictions, it represents 24 scientific organisations from 21 European countries and covers a geographical area the size of the USA with a similar scientific population. Its objective is to advance the science of medicinal chemistry by promoting cooperation and encouraging strong links between the national adhering organisations in order to promote contacts and exchanges between medicinal chemists in Europe and around the World.

EDITORIAL

Dear colleagues,

Modern drug discovery, similarly to other border disciplines, relies more and more on the availability, processing and mining of high quality data. Recent years have seen a growing availability of databases annotated with a variety of biological data, and for the first time academic researchers are beginning to have access to data generated under industry settings and standards. There is the risk, however, that the ability to generate data does not parallel the capacity to manage them, and, more importantly, to transform them into knowledge for medicinal chemists.
In this context, we publish in this issue of *MedChemWatch* a Perspective article originally published in the 2011 EFMC yearbook. In this perspective, Niklas Blomberg, Gerhard Ecker, Richard Kidd, Barned Mons, and Byrn Williams-Jones comments on the opportunity that the semantic web technologies are offering to the medicinal chemistry community, and present the example of the Open Pharmacological Concept Triple Store (OpenPHACTS) towards the creation of an open pharmacological space.

Continuing our presentation of leading European labs, we present in this issue the laboratory of Prof. Danijel Kikelj, at the Faculty of Pharmacy of the University of Ljubljana, Slovenia,

Gloria Cristalli, director of the ESMEC-Urbino, the EFMC-accredited European School of Medicinal Chemistry, reports on the 31st edition of the School, which has been held on July, 3-8.
The Second Summer School of Medicinal Chemistry, organized by the Spanish Society of Medicinal Chemistry has been granted this year as a EFMC event, and Maria Luz Lopez-Rodriguez and Javier Fernardez-Gadea report on the scientific outcome of the meeting.

As usual, you will find the columns on news from member societies and from the EC of the EFMC. Indeed, among the various and interesting events that will take place this year (and you will find the updated list in the 'EFMC events' section, as well as in the Meeting Calendar section of www.efmc.info) , the 4th edition of ASMC, which will be held in St. Petersburg, August 21-25, 2011

Gabriele Costantino, *Editor of MedChemWatch*

Knowledge Driven Drug Discovery goes Semantic

BY NIKLAS BLOMBERG, GERHARD F. ECKER, RICHARD KIDD, BAREND MONS, BRYN WILLIAMS-JONES*

While the availability of freely accessible information sources relevant to medicinal chemistry and drug discovery has grown over the past few years, the knowledge management challenges of this data have also grown enormously: how to get consistent answers, how to manage different interfaces, how to judge data quality, and how to combine and overlay the data to generate new knowledge. Open PHACTS (Open Pharmaological Concept Triple Store), a consortium of 22 partners, is poised to address this knowledge management challenge with semantic web technology to accelerate drug discovery. Here we describe the brief rationale, history and approach of the OpenPHACTS consortium with a final aim to create an Open Pharmacological Space (OPS).

Modern drug discovery research is increasingly dependent on the availability, processing and mining of high quality data. Analysis and hypothesis generation for drug-discovery projects requires careful assembly, overlay and comparison of data from many sources. For example, expression profiles and data from genome-wide association studies (GWAS)[1] need to be overlaid with gene and pathway identifiers and reports on compounds *in vitro* and *in vivo* pharmacologyUtility of data-driven research goes from virtual screening, HTS analysis, via target fishing and secondary pharmacology to biomarker identification.

Over the last 15 years industry has spend significant resources to integrate public data and information sources and align this with internal, proprietary data while the academic Medicinal Chemistry research community suffered from lack of access to large data sets, especially those including curated bioactivity data. In contrast to data from the bioinformatics world, where whole organism genomes, protein sequences, and protein structures are available to everyone, the chemoinformatics community traditionally is closed and proprietary. Access to commercial databases of high quality crystal structures and chemical information requires licenses, as do most of the software packages needed. Medium size and large sets of bioactivity data per se are rare, as large scale screening efforts have almost exclusively been performed in industrial laboratories. This has disconnected industrial and academic drug discovery efforts and directed academia more towards method development. Furthermore, *in silico* models developed in academia have largely been restricted to the small and scattered publicly available chemical space.

This setting changed drastically with the NIH roadmap, which led to the creation of PubChem, a public available depository of screening data. PubChem currently comprises 31 million compounds, 73 million substances and 490.000 bioassay results. Others like DrugBank, ChemBank, IUPHAR, and ChEMBLdb followed soon and today there is a panel of databases available which can be searched for compounds and associated biological data. The cur-

rent release of the ChEMBLdb contains more than 2,4 million activities of approx. 623.000 compounds measured against almost 7.200 targets.[2] The latest issue of the Nucleic acid research database summary lists almost 140 individual resources in the general field of molecular biology. However, there is still the urgent need for cleaning, improving and connecting these data to the public domain bioinformatics data, especially with respect to target validation, safety, efficacy and bioavailability. As an example, ChemSpider was set up as a free access platform for the aggregation, deposition and curation of community chemistry data, which has collected almost 25 million unique chemical structures linked out to over 400 data sources. ChemSpider has addressed the issues around data quality of chemical compound information available across the public data sources by running automated cleaning algorithms and providing wiki-like manual tools for commenting on and editing the aggregated compound information. Another milestone was the publication of the GSK 'Tres Cantos Antimalarial Compound Set', a set of 13 533 annotated compound structures shown to inhibit Plasmodium growth.[3] This for the first time allows academia to get access to a large data set derived under industry settings and standards and is likely to stimulate anti-malarial research through chemical biology and medicinal chemistry.

Public access to large amounts of information, by means of the open access policy for databases and papers, now will assist academia to contribute in a meaningful manner to drug discovery. Medicinal Chemists are thus expected to familiarize themselves with a multiplicity of highly variable sources and data formats, and their focus is shifting from data acquisition, to problem-solving skills, knowledge management and data integration.[4]

Nevertheless, there is a real danger that the high capacity to generate more data will not be in sync with our ability to manage the data well enough and, more importantly, to transform these data into biological and biochemical knowledge. Data integration over multiple sources is not sufficient to understand biology, but it is a prerequisite to even start to understand the complexity of any process in living organisms. As traditional medicinal chemistry research is embracing chemical biology and make increased use of phenotypic screening and high content biology for SAR, the requirements on data-analysis and integration will increase.[5] Unfortunately, this cumbersome and costly process is repeated across companies, institutes and academic laboratories. This represents a significant waste and an opportunity cost and effectively slows down scientific progress and consequently biomedical intervention.[6]

The emerging semantic web technologies and approaches are one way to address this major bottleneck in contemporary high throughput science. Simply put, "semantic web approaches" aims to establish unique identifiers for the concepts and entities within a given domain to allow effective connections to be made between data sources. More ambitiously unique identifiers are not only assigned to "things" (e.g. a compound) but also assigned to concepts such as "hydrolyses", "is a", etc (e.g "NaCl is a salt") to allow more advanced search and reasoning over large datasets. In the chemistry domain the CAS-number is an example of such a unique identifier; another one is the IUPAC InChI which rapidly gains popularity and support. As data volumes increase we would want to address increasingly complex search questions and rapid answers to questions such as "*provide all compounds which have been associated with liver toxicity and list their interaction profiles with the transporters expressed in the liver*" are becoming crucial for the success of drug discovery research programs. Currently, answering such a broad question requires cumbersome parsings, reading and integration efforts. The ideal situation would be an immediate answer to this question, with the full possibility to 'drill down' in the underlying information resources for deeper investigation.

The Concept Web Alliance (CWA), formed in 209 and comprising over 90 participants from academia and the private sector worldwide, is a collaborative community seeking to apply semantic concepts to deal with the massive amounts of information flooding the biological sciences and (later) other scientific disciplines. Many participants are also participants or members of other related networks and alliances, such as the W3C, the Pistoia Alliance and SageBionetworks, to name just a few. Collaboration of these like-minded alliances is a stated aim of CWA, which is built on the principles of Open Source, Open Access and Open Data. The rationale for the CWA semantic web approach is that classical data warehousing methods are no longer scalable to the size, spread and complexity of life science datasets, information resources and data analysis needs. These aims fit very well with the challenges already identified in harnessing public data for drug discovery.

A first step towards better global data integration and innovative ways to manage these data to produce meaningful information and finally knowledge is obviously the interoperability of the various data and information sets. Although standards are indispensible to this process, the *discussions about* standards can be lengthy and in fact may have an inherent potential side effect of blocking the very process it aims to accelerate. The consequences of not agreeing to common standards are evident when looking on public bioactivity data bases such as PubChem, BindingDB, and DrugBank. All of them host a broad range of pharmacological activity data, mostly manually curated, which are accessible through various web-based tools. However, the lack of common standards for representation of these data makes it excruciatingly time consuming to exploit the information present. Nevertheless, in a fully connected world where many different teams are providing valuable, but specialist, data-sources top down approaches as e.g. previously enforced by IUPAC for chemical nomenclature, will most likely fail in the biomedical domain. As an example, the CWA has adopted the approach of 'bottom up standard setting by best practices'. Recognizing that the power of standards lies in their widespread adoption the CWA firmly believe that the only long-term sustainable model for a scientific system to support global computational biology approaches as needed is full openness around the core semantic components, vocabularies and interfaces. However, this does not preclude the exposure and the delivery of proprietary content, nor does it preclude value-added closed-source or commercial services delivered on top of this system.

In order to succeed and gain widespread community adoption, this approach will need to go way beyond the current state of the art of tools in the life sciences and semantic web domain. The transition from classical, hypothesis driven research towards systems approaches requires rigorous new methodology. A further key challenge is that current data sources are largely incompatible with massive computational approaches and the vast majority of drug-discovery sources cannot easily interoperate. Recently developed data and text mining approaches, improved data capture standards, and leveraging semantic web technology open a first-time-opportunity to achieve interoperability through the semantic harmonization of data in key data sources. A priori data interoperability 'at the source' would therefore be a desired long-term effect of this distributed approach. Regarding questions around long-term sustainability of available resources, recent studies in the scope of the ELIXIR project have shown that out of 531 databases surveyed, 63 were either not online anymore or had not been updated since 2005 and, for a further 78, the update status was unclear. More importantly, less than 10% of the biomolecular resources surveyed indicated that they had multi-annual funding secured. The data resource landscape is therefore very fragile and a large and influential consortium involving academic as well as industrial drug-discovery partners can play an important role in capturing the most important 'assertional content' globally in a stable, interoperable and sustainable format.

The semantic approach, is based on the extraction and encoding of free-text, table, image, molecular sequence and structured information in Resource Description Framework (RDF) assertions that together with provenance data to form the basic building block of interoperability. The concept of RDF "triple"s (extracted simple assertions, also called nanopublications by CWA) has already been adopted by a wide and rapidly expanding community and is being implemented both for bioinformatics and chemogenomics. For instance, the Bio2RDF.org project aims to transform different sources of bioinformatics data into a distributed platform for biological knowledge discovery.[7] Initially, the authors focused on building a public database of open-linked data with web-resolvable identifiers that provides information about named entities. This involved the conversion of open data represented in a various formats to RDF-based linked data with normalized names. Bio2RDF entities also make reference to other open linked data networks thus facilitating traversal across information spaces. Bio2RDF is currently indexing around 5 billion triples, and is built with the open source Virtuoso database. However, currently the redundancy problem is not yet handled in Bio2RDF and in the linked open "data-cloud" in general. One step further is the Chem2Bio2RDF initiative, which comprises a repository aggregating data from multiple chemogenomic data sources that is cross-linked to Bio2RDF. Chem2Bio2RDF also includes a tool to facilitate query generation as well as a set of extended functions to address specific chemical/biological search needs. Potential usefulness in specific examples of polypharmacology, multiple pathway inhibition and adverse drug reaction–pathway mapping has been demonstrated.[8] Another very valuable source recently launched

is ChemProt (www.cbs.dtu.dk/services/ChemProt/), a disease chemical biology database, which is based on a compilation of multiple chemical–protein annotation resources, as well as disease-associated protein–protein interactions (PPIs).[9] ChemProt comprises more than 700.000 unique chemicals with biological annotation for 30.578 proteins, leading to more than 2 million chemical–protein interactions, which were integrated in a quality scored human PPI network of 428.429 interactions. ChemProt can assist in the *in silico* evaluation of environmental chemicals, natural products and approved drugs, as well as the selection of new compounds based on their activity profile against most known biological targets, including those related to adverse drug events. Nevertheless, the increasing availability of linked data sources also requires innovative browsing and navigation tools, such as iPHACE (cgl.imim.es/iphace/).[10] iPHACE represents an integrative web-based tool to navigate in the pharmacological space defined by small molecule drugs contained in the IUPHAR-DB, with additional interactions present in PDSP. Extending beyond traditional querying and filtering tools, iPHACE offers a means to extract knowledge from the target profile of drugs as well as from the drug profile of protein targets.

Open Pharmacological Space

In light of all these developments and in order to foster public-private partnership the Innovative Medicines Initiative launched a call for development of an Open Pharmacological Space to establish a set of practical standards for the major public drug discovery resources and to implement these standards in a public infrastructure to the benefit of both pharma and academic drug-discovery communities.

Open PHACTS, the winning consortium, will concentrate on a semantic web approach to develop an open source, open standards and open access innovation platform (OPS). The Open PHACTS project will be one of the first international attempts to create a reliable and scalable system, a common product beyond collective prototyping. OPS aims to deliver a sustainable, reliable web based environment through proven agile software engineering models. OPS will comprise data, vocabularies and infrastructure needed to accelerate drug-oriented research. This semantic integration hub will address key bottlenecks in small molecule drug discovery: disparate information sources, lack of standards and shared concept identifiers, guided by well defined research questions assembled from participating drug discovery teams. Workflows for data capture, processing, interoperability, visualization, and chemogenomics will be developed to create a comprehensive Systems Chemical Biology Analysis Network. Security issues around proprietary data, shared via the CWA nanopublication system and accessible for safe querying and reasoning will be properly addressed with expert trusted parties. The core Open PHACTS consortium comprises 14 European core academic and SME partners as well as 8 EFPIA members, with leading experts in the fields of data mining, annotation, small molecule data storage and manipulation, target related bioinformatics, RDF-type information handling, massive *in silico* reasoning and chemical biology. Noteworthy, Open PHACTS is not only open in terms of data but also in terms of the consortium itself. With the alignment of other Knowledge Management projects in IMI and a wider community of like-minded partners it is likely that already in 2011 the approach taken by Open PHACTS will be actively followed, co-developed and implemented by close to 100 partners world-wide. Any partner with an interest and an ability to contribute data, software or expertise is principally considered as an 'associated partner'.

Dissemination and community engagement will also utilize the manifold channels EFMC and RSC can provide. A large and influential consortium like this, involving academic groups, learned societies, as well as industrial drug-discovery partners collaborating in the context of OPS is likely to increasingly drive researchers around the globe to capture and distribute data and information in a semantically interoperable and computer readable format, as their data will ‹connect› and ‹mean› more from the onset. We therefore emphasize that - if successful and sustainable – the OPS project is likely to significantly contribute to more successful and cost-effective development of drugs and vaccines in human and animal health, as well as in nutrition and personal genomics. Turning data into knowledge is the cornerstone of successful drug discovery, but is the core business of science in general. A future driven by the open sharing of data, tools, services and workflows benefits the whole scientific community.

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The Medicinal Chemistry Programme Group

University of Ljubljana, Faculty of Pharmacy, Slovenia

DANIJEL KIKELJ

Mission of the programme group *Medicinal Chemistry* at the University of Ljubljana - Faculty of Pharmacy (http://www.ffa.uni-lj.si/en.html)), leaded by Danijel Kikelj and comprising several research labs, is a high-quality research in medicinal chemistry directed towards discovery of novel biologically active compounds for human health. In order to fulfil this mission, the programme team is engaged in design, synthesis and biological evaluation of bioactive compounds, in development of new approaches to drug design and synthesis, and in development of novel molecular tools for studying the action of bioactive compounds on molecular level.

The programme group, financed by grants from the Slovenian Research Agency (http://www.arrs.gov.si/sl/), is becoming increasingly engaged in EU projects. The Framework 6 project **INTAFAR** (*Inhibition of New Targets for Fighting Antibiotic Resistance*), aiming at better understanding of the physiology and biochemistry of bacterial cell morphogenesis and peptidoglycan biosynthesis was successfully finished in 2010 (http://www.eur-intafar.eu/). In 2010 the programme group started with a 4-year FP7 EU collaborative project *Exploring Marine Resources for Bioactive Compounds: From Discovery to Sustainable Production and Industrial Applications* (**MAREX**) in which marine bioactive compounds are being used as leads for drug design (http://www.marex.fi/). In 2011 the programme team started with the FP7 EU project **ORCHID** (*Open Collaborative Model for Tuberculosis Lead Optimization*) which will encompass the parallel progression of the three anti-tubercular compound families through lead optimization and MoA studies for whole cell inhibitors and the optimization of an InhA inhibitor for later preclinical development (http://cordis.europa.eu/home_en.html).

The interdisciplinary conceived research programme *Medicinal Chemistry* which is based on a uniform concept which comprises (*i*) understanding the biomolecular basis of disease and (*ii*) knowing the 3D structure of biological macromolecules (enzymes, receptors) involved in particular disease, is focusing on (a) rational design and discovery of drug molecules exerting their action on validated biological targets, (b) their synthesis and (c) biological evaluation aiming at discovery of innovative medicines with *antimicrobial* and *antiviral*, *antithrombotic* and *antitumour* activity. A new paradigm of designed multiple ligands targeting two or more biological macromolecules is being applied as an innovative approach to the design of antithrombotic, antibacterial and antitumour drugs. A constituent part of the programme is genomic research which is concentrating on studying influence of compounds, designed and prepared following the outlined concepts, on expression and interactions of proteins in the cell. The aims of this strategy are new innovative bioactive compounds with a potential to be developed to drugs and understanding of their complex action on protein network in the cell.

With the aim of achieving therapeutical benefit in bacterial, viral, thrombotic and cancer diseases, our research is concentrated on *(i) bacterial enzymes involved in intracellular steps of peptidoglycan biosynthesis and enzymes which are antitubercular targets* (*ii*) *enzymes involved in the process of blood coagulation and other serine proteases involved in apoptosis* (*iii*) *enzymes involved in metabolism of steroid hormones,* (*iv*) *fibrinogen*

and vitronectin receptors and (*v*) *receptor DC-SIGN of dendritic cells*. The dogma of achieving the possibly highest selectivity on particular target still prevailing drug design is being critically confronted with emerging concept of **designed multiple ligands** which achieve better therapeutic effect by simultaneous modulation of several target macromolecules. Combination of enzyme inhibitory action and receptor modulation activity in a single molecule with the aim of achieving therapeutical benefit represents an outstanding challenge for the research programme. The first successful steps towards integration of receptor antagonist and enzyme inhibitor in the same molecule, still being in the initial stage worldwide, has been already done by our group in antithrombotic compounds and we are striving to develop this concept into an established strategy also in other therapeutic fields. For rational design of drugs targeting particular biological macromolecules we are using **molecular modeling tools** and developing a concept of **mimicking biologically active peptides, sugars and lipids** with peptidomimetics, glycomimetics and lipidomimetics, which still remains a leading strategy in drug design starting from natural lead compounds.

Based on the presented uniform concept, the programme comprises the following main research topics:

Inhibitors of peptidoglycan biosynthesis

The biosynthesis of peptidoglycan is a complex process which is carried out in three distinct cell phases (cytoplasmic, membrane and periplasmic) and which involves over 20 enzymes. Due to the essential character of peptidoglycan, action of specific inhibitors of its biosynthesis during bacterial growth rapidly leads to the destructuration of the envelope and to cell lysis. The numerous enzymes involved in this biosynthetic pathway thus constitute potential targets for the search for new antibacterial drugs. Several inhibitors of biosynthesis of the peptide part of peptidoglycan, catalyzed by *Mur ligases* (MurC, MurD, MurE and MurF) as well as *D-alanine-D-alanine ligase* (Ddl), have recently been designed and synthesized by our programme group (Figure 1). We try to apply the *multiple inhibition concept to ATP-dependant Mur enzymes* with a hope that a succesful inhibition of ATP binding to the ATP-binding site could, if a problem of selectivity against other ATP-dependant enzymes such as human kinases would be successfully solved, lead to effective universal chemoterapeutics.

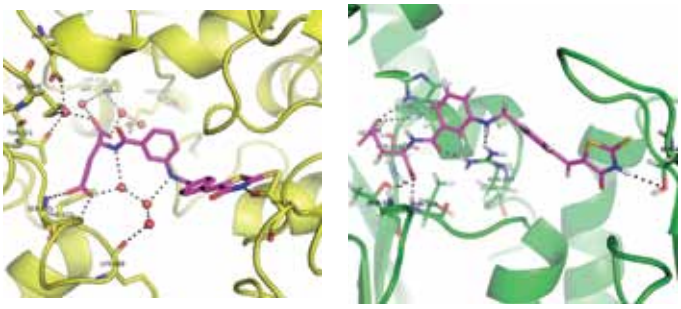

Figure 1. X-ray binding mode of dual inhibitor (IC50 S. aureus MurD = 8,2 mM; IC50 S. aureus MurE = 17,5 mM) possessing antibacterial activity (MIC S. aureus and MRSA = 8 mg/mL) (in magenta) in the active site of MurD (PDB ID code: 2Y1O) and GOLD-calculated conformation of the same inhibitor in MurE model active site (in magenta). Hydrogen bonds between dual inhibitor and MurD and MurE active site residues or crystal water molecules (in red) are presented as dashed lines (Tomašić et al., unpublished results).

Selected recent publications:

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Antagonists of receptor DC-SIGN as potential antibacterial and antiviral compounds

DC-SIGN (Dendritic Cell-Specific ICAM-3 Grabbing Non-integrin) is a C-type lectin implicated in the recognition of pathogens and in some of the earliest stages of the infection

process. Certain pathogens exploit DC-SIGN in order to bind immune system cells, but circumvent the processes of internalization and degradation. DC-SIGN is thus used as a Trojan horse to invade lymphocytes T $CD4^+$, which is the main HIV invading mechanism. Recently we have designed, synthesized and biologically evaluated several families of DC-SIGN antagonists and developed an assay that measures inhibition of human dendritic cell adhesion on mannan-coated microtiter plates, suitable for screening a large number of compounds, determination of inhibitory constants (IC50) and fast discovery of new DC-SIGN antagonists.

Recent publications:

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Inhibitors of steroid hormone metabolism as potential antitumour drugs

Steroid hormones play an important role in the aetiology of hormone-dependent diseases, such as breast, prostate and endometrial cancer, disorders of reproduction, and neuronal diseases. The occupancy of the steroid hormone receptors is regulated mainly by hydroxysteroid dehydrogenases, which convert steroids at positions 3, 11, 17 and 20 of the steroid core, thereby acting as molecular switches. The 17β-hydroxysteroid dehydrogenases (17β-HSDs) modulate the biological potencies of estrogens and androgens by converting inactive 17-keto-steroids into their active 17β-hydroxy-forms (such as estradiol, testosterone and dihydrotestosterone), or vice versa. These enzymes play a key role in hormonal regulation and function in the human and represent emerging therapeutic target for the control of estrogene- and androgene-sensitive cancers. Recently we have discovered that simple coumarines prepared by Suzuki-Miyaura cross coupling reaction significantly inhibit 17β-HSD1 in a recombinant enzyme assay with high selectivity over 17β-HSD2. The best inhibitors in series were 7-phenyl-3-acetyl coumarin derivatives with the most potent compound having IC50 value of 268 nM and good selectivity over 17β-HSD2 receptors.

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Coagulation enzymes inhibitors and modulators of fibrinogen receptor as novel antithrombotic compounds with dual action

In order to achieve a synergistic antithrombotic effect, simultaneous application of anticoagulant and antiaggregatory drugs (e.g. thrombin inhibitors and fibrinogen receptor antagonists) is frequently applied in clinical practice. Complementary structures of pharmacophores D-Phe-Pro-Arg of thrombin inhibitors and Arg-Gly-Asp of fibrinogen receptor antagonists inspired us to merge both pharmacophores in a low-molecular weight peptidomimetic compounds which inhibit thrombin and act as antagonist of fibrinogen receptor, thus displaying anticoagulant and antiaggregatory activity. Optimization of a class of compounds afforded dual antithrombotic compounds possessing a well balanced activity on both (Figure 2). The best classes of antithrombotic leads with dual function were found to possess antioxidative and radical scavenging activity which synergistically contributes to their antithrombotic potential.

Selected publications:

1 Ilić M, Kontogiorgos C, Hadjipavlou-Litina D, Ilaš J, Kikelj D. Thrombin inhibitors with lipid peroxidation and lipoxygenase inhibitory activities. *Bioorg Me. Chem Lett* **2011,** doi: 10.1016/j.bmcl.2011.06.089.
2 Ilaš J, Jakopin Ž, Borštnar T, Stegnar M, Kikelj D. 3,4-Dihydro-2H-1,4-benzoxazine derivatives combining thrombin inhibitory and glycoprotein IIb/IIIa receptor antagonistic activity as a novel class of antithrombotic compounds with dual function. *J Med Chem* **2008,** 51, 5617-5629,
3 Ilaš J, Tomašić T, Kikelj D. Novel potent and selective thrombin inhibitors based on a central 1,4-benzoxazin-3(4H)-one scaffold. *J Med Chem* **2008,** 51, 2863-2867.
4 Štefanić P, Anderluh M, Ilaš J, Mravljak J, Sollner Dolenc M, Stegnar M, Kikelj D. Toward a novel class of antithrombotic compounds with dual function. Discovery of 1,4-benzoxazin-3(4H)-one derivatives possessing thrombin inhibitory and fibrinogen receptor antagonistic activities. *J Med Chem* **2005,** 48, 3110-3113.

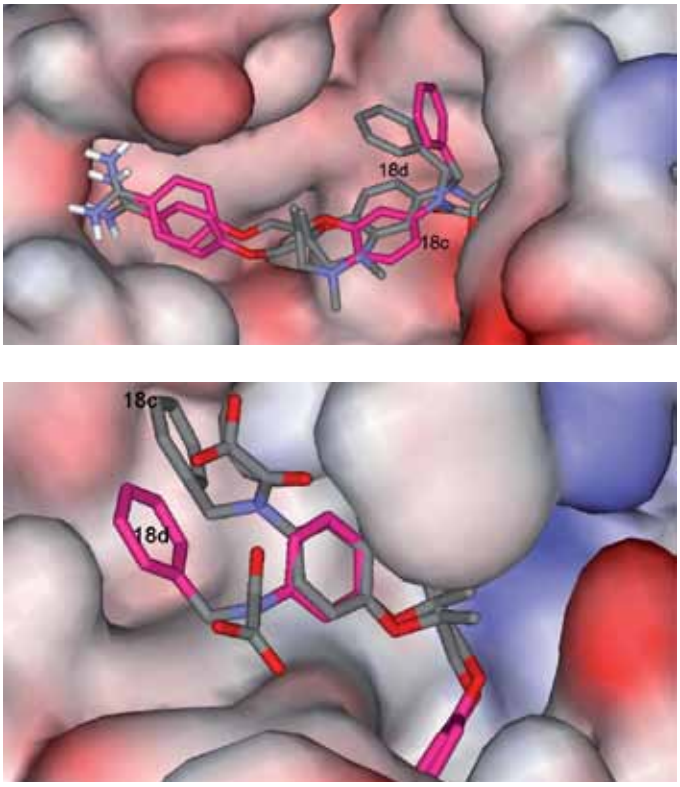

Figure 2. Dual antithrombotic compounds (R)-18c and (R)-18d docked in the active site of thrombin (top) and GPIIb/IIIa binding site (below).

Nitroxide-fluorophore double probes

Study of the transmembrane signal transduction mechanism with non-destructive spectroscopic methods [electron paramagnetic resonance (EPR) and fluorescence spectroscopy/microscopy (FS)] is connected with progress in appropriate molecular tools – spin-labels, fluorescence-labels and dual probes. To study extra cellular surfaces, cell interactions with its surrounding and influence of cholesterol oxidized products on membrane domain structure, we try to develop labelled glycomimetics and lipidomimetics which will enable efficient exploitation of all possibilities of non-destructive spectroscopic methods like EPR and FS. A further focus of our research is on design and synthesis of labelled glycomimetics and lipidomimetics with preserved biological activity of non-labelled parent molecule. A special attention is focused on design and synthesis of dual labelled molecular probes that combine paramagnetic nitroxide group and fluorophore. We expect that dual probes will enable simultaneous application of two non-destructive spectroscopic (EPR, FS) techniques and thus make possible more profound understanding of membrane processes.

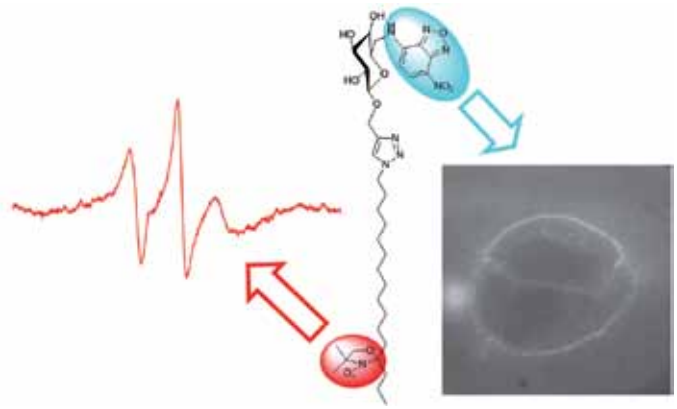

Figure 3. Nitroxide-fluorophore double probes: a potential tool for studying membrane heterogeneity by ESR and fluorescence.

Selected publications:

1 Pajk S, Garvas M, Štrancar J, Pečar S. Nitroxide-fluorophore double probes: a potential tool for studying membrane heterogeneity by ESR and fluorescence. *Org Biomol Chem* **2011**, 9, 4150-4159.
2 Humar M, Ravnik M, Pajk S, Muševič, I. Electrically tunable liquid crystal optical microresonators. *Nature Photonics* **2009**, 3, 595-600.
Pajk S, Pečar S. Synthesis of novel amphiphilic spin probes with the paramagnetic doxyl group in the polar region. *Tetrahedron* **2009**, 65, 659-665.
3 Mravljak J, Pečar S. A new glucosamine-containing amphiphilic spin probe. *Tetrahedron Lett* **2009**, 50, 567-569.

Group Members

Danijel Kikelj, Stanislav Gobec, Marija Sollner Dolenc, Aleš Obreza, Lucija Peterlin Mašič, Anamarija Zega, Marko Anderluh, Jožko Cesar, Janez Ilaš, Janez Mravljak, Matej Sova, Rok Frlan, Žiga Jakopin, Matej Živec, Samo Turk, Nace Zidar, Tihomir Tomašič, Roman Šink, Stane Pajk, Irena Mlinarič Raščan, Nataša Karas Kuželički and Damjan Janeš.

For a complete bibliography of the programme group in the last 3 years see **http://izumbib.izum.si/bibliografije/P2011072114475O-P1-0208.html**

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EFMC NEWS & EVENTS

BY NELE COULIER AND KOEN AUGUSTYNS

EFMC is very proud to announce the launch of its brand new website! A modern design and structure together with an interesting, up to date content makes the site interesting and attractive for the medchem community. We invite you to have a look at www.efmc.info, to find out more on the numerous activities of EFMC. We encourage any feedback from users of the site. Please feel free to email the Administrative Secretariat (administration@efmc.info) with your recommendations.

Join us on LinkedIn! Become member of the EFMC LinkedIn group and stay updated on EFMC activities. As the group becomes populated, this will create a unique online forum for medicinal chemistry.

The third edition of "Frontiers in Medicinal Chemistry – Emerging Targets, Novel Candidates and Innovative Strategies" has been organised on June 19-21 in Stockholm together with the Swedish Academy of Pharmaceutical Sciences and the Medicinal Chemistry Division of the American Chemical Society. Following the spirit of this series, it brought together top quality speakers from the Scandinavian region and from the US, and attracted more than 250 participants. A report of the meeting is available under "EFMC events".

Together with Maurizio Botta and Ulrike Holzgrabe, Gerhard Ecker organised two EFMC-sponsored sessions on "Innovative Strategies to Combat Neglected Diseases" at PharmSciFair 2011, held in Prague on June 13-17. EFMC was highly pleased with the quality of the contributions from Simon Croft, Maria Laura Bolognesi, Reto Brun, Oludotun A. Phililps, Franz Bucar and Anthony Williams.

At the EFMC Council meeting, held on June 19 in Stockholm on occasion of the Frontiers in Medicinal Chemistry, the Council elected Phil Jones (UK) as new member of the Executive Committee. From January 1, 2012 on Phil Jones will replace Javier Fernandez (Spain).

EFMC ORGANISED EVENTS

4th International Symposium on Advances in Synthetic and Medicinal Chemistry
August 21-25, 2011, St-Petersburg (RUS)
http://www.asmc11.org

4th EFMC Short Course on Medicinal Chemistry – Safety and Attrition
December 7-9, 2011, Oegstgeest (NL)
http://www.ldorganisation.com

EFMC SPONSORED EVENTS

4th BBBB International Conference on Pharmaceutical Sciences
September 29-October 1, 2011
Bled (SLO)
http://www.bbbb-eufeps.org/

29th Cyprus-Noordwijkerhout-Camerino Symposium
October 2-7, 2011, Limassol (CY)
http://www.quintessence.com.cy

Annual One Day Meeting on Medicinal Chemistry At SRC & KVCV: "Drug Design Against Emerging Targets: Opportunities and Challenges"
November 25, 2011, Ghent (B)
http://www.ldorganisation.com

EFMC Sponsored Session on Oncology at the AFMC Meeting 2011
Nov. 29-Dec. 2, 2011, Tokyo (J)
http://www.aimecs11.org/

30th Noordwijkerhout-Camerino-Cyprus Symposium
May 13-17, 2012, Amsterdam (NL)
far@few.vu.nl

EFMC Sponsored Session at the 4th EuCheMS Chemistry Congress
August 26-30, 2012
Prague (CZ)
http://www.euchems-prague2012.cz/

EFMC SPONSORED SCHOOLS

6th Summer School on Drug Design
September 11-16, 2011, Vienna (A)
http://summerschool.europin.at

Summer School on Pharmaceutical Analysis (SSPA)
September 19-21, 2011, Pavia (I)
http://chifar.unipv.it/sspa2011/

20th LACDR School on Medicinal Chemistry
October 25-28, 2011
Oegstgeest (near Leiden) (NL)
http://medchem.lacdr.gorlaeus.net/node/3039

2nd Edition of the SEQT Summer School on "Medicinal Chemistry in Drug Discovery: The Pharma Perspective"

BY MARÍA LUZ LÓPEZ RODRÍGUEZ
SILVIA ORTEGA GUTIÉRREZ
JAVIER FERNÁNDEZ GADEA

REPORT

The second edition of the SEQT Summer School on "Medicinal Chemistry in Drug Discovery: The Pharma Perspective" has become a major success. It took place in San Lorenzo de El Escorial (Madrid, Spain) on 26-29 June, 2011. This second edition of the Summer School, an event sponsored by the European Federation of Medicinal Chemistry (EFMC), was organized by the Spanish Society of Medicinal Chemistry (SEQT) and Janssen with the aim of approaching the pharma industry to young researchers, both graduate students and post-doctoral associates working in the chemistry and health sciences related fields.

During the three days of the school, 65 participants coming from seven different countries around the world gathered together in the first-class facilities of Euroforum-Felipe II. The attendants (30% of whom were from the industry and the remaining 70% came from academia) had the opportunity to learn about the latest research trends in pharmaceutical drug discovery and development illustrated through real case studies led by an exceptional panel of industry experts currently working at international pharma industries.

The School started on with the opening session led by Prof. María L. López-Rodríguez (SEQT President), Dr. Javier Fernández-Gadea (Director of Basic Research at Janssen Spain) and Prof. Gabriele Costantino (EC member, representing EFMC). Then, during three intense days, an enthusiastic teaching team, composed by Kristof van Emelen (Janssen), Mark Bunnage (Pfizer), Jordi Gràcia (Almirall), Víctor Rubio (Faes Farma), Rob Young (GlaxoSmithKline) and José Cid (Janssen) handled different case studies in a very interactive manner fostering the discussion among the participants, organized during all the school in several work-teams. The sessions covered a number of topics dealing with the different stages of modern research and development in industry. Among them, the speakers considered essential aspects about target selection and hit design and development, with a special emphasis on the pharmacokinetic properties. Also, the importance of the scale-up and production processes was also highlighted.

The participants rated both the teachers and the information they provided very high (an average of 4.65 out of 5.00). The open interactive atmosphere was deeply appreciated. The inclusion of questions during the cases studies as well as sessions with questions and problems based on the preceding talks was extremely successful. In addition to the case studies, two poster sessions gave the opportunity to the attendants to present their works and to discuss with the teachers and the senior participants the most significant aspects of their research. In addition, the teachers together with the organizing and scientific committee selected 15 posters to be presented as short oral communications by the young researchers. These sessions were also highly valued by the participants.

The venue, conveniently located close to Madrid (in the pleasant village of San Lorenzo de El Escorial), was Euroforum Felipe II. The place was originally built as a luxury hotel and situated in a privileged residential area, among the forest and half-way up the Abantos massif. Today it has been turned into the modern and comfortable Executive Development Centre.

All in sum, the motivating scientific environment during the sessions and the friendly and informal atmosphere, together with the careful organization and the availability of the teachers throughout the school, were highly appreciated by the participants who praised the school as highly productive, interesting and formative event.

The XXXI Edition of the European School of Medicinal Chemistry (ESMEC) has successfully been held in Urbino (Italy)

BY GLORIA CRISTALLI

REPORT

The XXXI edition of the European School of Medicinal Chemistry (ESMEC) has been held as usual in the Renaissance scenario of Urbino from July 3 to July 8, 2011. Of a total of 160 participants who have attended the this years edition, more than 65 % was constituted by PhD, master of post-doctorate students, 20 % by researchers from the academia and 15 % by researchers from industry. Although the participation to the School is a requirement for many Italian doctorate programs in medicinal chemistry, and thus the majority of the registrants came from Italy, the about 20 % of non Italian participants is an indication of the growing interest that the School is gaining around Europe. Interest that this year was particularly pushed by the appealing scientific program, by the quality of the invited speakers, and by some fellowships offered by the School, by EFMC, and by Farmindustria. In line with the well established format based on a four daily sessions, this year the School has covered the following topics: Infectious Diseases: Bacterial and Mycobacterial Infections. The Problem of Bacterial Resistance; Protein-Protein Interactions in Drug Discovery; Organo- and Bio-Catalysis in the Synthesis of Bioactive Compounds; Hot Topics.

The first session on Bacterial and Mycobacterial Infections has seen Alan Kozikowski (University of Illinois, USA) and Gian Maria Rossolini (University of Siena, I) introducing the misuse of antibiotics and the rise of bacterial resistance as a major driver of unmet clinical needs. In fact, despite the successes of the antibacterial chemotherapy, resistance to several antibiotic classes began to emerge in Gram-positive bacteria in the United States during the 1990s. The emergence of multidrug-resistant strains of S. pneumoniae, Enterococcus faecium, and S. aureus emphasizes the critical need to develop novel antibiotics to treat serious Gram-positive infections. In the second half of the session, Sergio Lociuro (THOT consulting Sagl, Maroggia, CH) has focused on new approaches to fight against bacterial resistance like optimising "old" classes, searching new classes acting on "old" targets, searching new classes acting on never exploited targets, preferring broad spectrum agents vs. narrow spectrum vs. single pathogen agents. Furthermore, Alan Kozikowski, with a second lecture on this topic, has illustrated the use of high throughput screening (HTS), medicinal chemistry, and cell biology in the discovery of new drugs against resistant strains of TB.

The second session was devoted to Protein-Protein Interactions (PPIs) in Drug Discovery and provided participants with an up-to-date overview of fundamental concepts and strategies, as well as biophysical and computational approaches and tools in a field of paramount importance. The first speaker, Kumlesh Dev (Trinity College Dublin, IR), focused his talk on the new concept of generating compounds that alter receptor function from the inside (i) of the cell by regulating intracellular (i) trafficking; in other words, on the discovery of i-agonists and i-antagonists, where the "i" refers to inside and intracellular regulation. The second speaker, Domenico Raimondo (University "La Sapienza", Roma, I), presented computational approaches for studying protein-protein interactions such as protein modeling, genome functional annotation, protein structure analysis and characterization of protein-protein and protein-DNA complexes. The last two lectures given by Alessandro Padova (Siena Biotech, I) and Kristian Strømgraard (University of Copenhagen, DK) have focused the possibility of modulating protein-protein interactions to find new therapies for cancer and neurological disorders or chronic neurodegenerative diseases.

The third session on Organo- and Bio-Catalysis in the Synthesis of Bioactive Compounds has seen the presentation of very interesting approaches and methodologies in organic synthesis directed to potential drug molecules. Paolo Melchiorre (Institute of Chemical Research of Catalonia, Tarragona, E) in the opening lecture has addressed the emerging field of aminocatalytic cascade reactions that recently proved to be a new strategy to recreate the intricate structural scaffold and related complex stereochemistry of natural-like compounds with very high fidelity. The second talk, given by Marco Bella (University "La Sapienza", Roma, I) was strictly connected to the previous one since it has given an overview of the asymmetric organocatalysts which act without the formation of any covalent bond to the substrate. The third lecture, by Marco Bandini (University of Bologna, I), has illustrated the advantages

of the synthesis of complex molecules provided by a combination of the organo- with organometallo-catalysis. The last two lectures have been dedicated to biocatalysis. Kurt Faber (University of Graz (A) has presented the application of ene-reductase-mediated asymmetric synthesis to the preparation of several different bioactive compounds, whereas Roland Wohlgemuth (Sigma-Aldrich, Buchs, CH) ha given an overview of biocatalytic transformations in the context of the growing importance of metabolites as drugs, drug-derived products, analytical standards, tools for elucidating biochemical pathways and for metabolomic studies.

The last day has covered some hot topics. More in detail, recent progresses in the structure and function of ion channels, transporters and G-protein coupled receptors have been illustrated by Chris Ulens (Laboratory of Structural Neurobiology, Leuven, B) who showed how the several three-dimensional structures of GPCR, ion channels and transporter now available may help the design of specific modulators. Olivier Bezencons (Actelion Pharmaceuticals Ltd, Allschwil, CH), starting from Aliskiren, the first Direct Renin Inhibitor (DRI) clinically available, presented the discovery of a new class of DRI with a piperidine-based structure; one of these compounds, ACT-077825 is presently in clinical trials for the treatment of hypertension. Henk Stunnenberg (Radboud University, Nijmegen, NL) showed how the systems biology approach, which considers the cell as a system whose components interact in a certain way in normal conditions or in response to a chemical or genetic perturbation, can be applied to find treatments for leukemia. The last speaker of this edition was Nicola Curtin (University of Newcastle upon Tyne, UK). She focused her talk on poly(ADP-ribose) polymerases (PARPs) that are enzymes activated by DNA strand breaks and involved in DNA repair and on the application of PARP inhibitors in cancer therapy. In fact they are one of the first classes of compounds that interact in a synthetic lethal manner with mutations in the genes encoding proteins involved in DNA repair. Some PARP inhibitors, are now in clinical trials for BRCA1 or BRCA2 mutants tumors, for triple-negative breast cancer, ovarian cancer and other solid tumors.

The didactic program of the School was completed by two workshops on protein-protein interactions in drug discovery and on organo- and bio-catalysis in the synthesis of bioactive compounds, promoting a closer interaction between students and lecturers and among students with different background and know-how. Furthermore, the PhD students following the last year of PhD course and them coming from foreign countries have been invited to present a poster on their research during two poster sessions, where results and methodologies have been freely discussed and the 10 best posters have been selected for an oral presentation.

A very interesting part of the School was a round-table organized by Farmindustria, the Italian association of pharma industries, to discuss on 'Medicines and Public Private Partnerships: From Labs to Patients'. The meeting has seen a large and active participation of young researchers and PhD students.

As confirmed by the analysis of the evaluation questionnaires completed by participants, the School has certainly achieved its scientific and didactic aims, thus confirming the success of a format that nicely mixes up advanced seminars and didactic introductions and workshops. The informal environment and the appealing social program have also contributed to promote a productive interchange between participants. In conclusion, the Scientific Committee hope that ESMEC-Urbino school could contribute to keep at a very high level the didactic offer of the EFMC. With the hope to continue along this way, the organizers are looking forward to seeing you in Urbino for the XXXII edition, in July 2012.

News from the Societies

BY ERDEN BANOGLU

THE BIOLOGICAL AND MEDICINAL CHEMISTRY SECTOR OF THE RSC

Malcolm Campbell Memorial Prize 2011

The Biological and Medicinal Chemistry Sector of the RSC is proud to announce the winner of the Malcolm Campbell Memorial Prize for 2011. The prize has been awarded to the Liverpool team of Paul M. O'Neill, B. Kevin Park and Stephen A. Ward for work in the area of antimalarial drug discovery and chemical biology of Plasmodium falciparum.

The Malcolm Campbell Memorial prize commemorates Professor Campbell's outstanding contributions in a broad range of chemistry and their applications to the understanding of bioactivity. The prize is awarded biennially and the 2011 prize will be formally presented to the winning team during the RSC/SCI Medicinal Chemistry Symposium to be held in Cambridge, 11th-14th September 2011.

The BMCS Committee wishes to express its gratitude for the high quality entries from both academia and industry for the 2011 award. Details of the Award may be found here [http://www.rsc.org/Membership/Networking/InterestGroups/BMCS/Activities/CampbellAward.asp] and details of forthcoming RSC-BMCS events may be found here: http://www.rsc.org/Membership/Networking/InterestGroups/BMCS/ForthcomingEvents.asp.

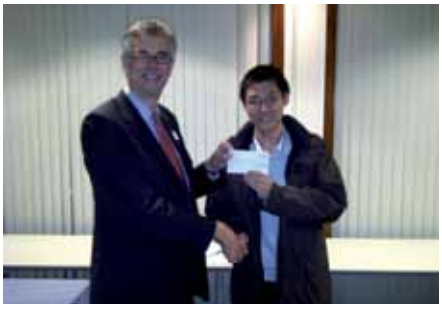
BMCS Postgraduate Symposium for Biological and Medicinal Chemistry

10th December, 2010 at the Chemistry Department, Cambridge University

The Biological and Medicinal Chemistry Sector (BMCS) Postgraduate Symposium on Biological and Medicinal Chemistry was held in the Department of Chemistry at the University of Cambridge on Friday 10th December 2010. This annual symposium for PhD and postdoctoral students working in biological chemistry, medicinal chemistry, or related areas event aims to provide students working in these fields with an opportunity to present their research work in public and also to learn a little about the drug discovery and development process. The programme included keynote lectures by Professor Barry Potter from the School of Pharmacy at the University of Bath, one of the winners of the 2009 Malcolm Campbell Award, Dr Steve Lindell from Bayer CropScience in Germany and Dr Matt Tozer from Peakdale Molecular. There is no registration fee for the symposium which was attended by 140 students from across the UK as well as one participant from Italy and one from the USA.

There were also nine oral presentations and 20 poster presentations from students, whose work covers cutting edge research in the areas of biological chemistry and drug discovery, potentially leading to advances which could positively influence the future of drug treatment. Prizes were awarded for the best presentations with the oral prize going to Zhiyong Yu from Imperial College for his work titled 'Design and synthesis of Inhibitors for Plasmodium falciparum N-MyristoylTransferase: a promising target for antimalarial drugs' while the poster prize went to Rebecca Nonoo, also from Imperial College, for her work titled 'Towards kinetic template-guided tethering of fragments'

Advance notice: the 2011 symposium will be held in the Department of Chemistry at the University of Cambridge from 1000 to 1800 on Friday 9th December 2011.



Zhiyong Yu from the Department of Chemistry, Imperial College, winner of the oral presentation prize at the symposium, being presented with his cheque for £250 by Professor Barry Potter from the School of Pharmacy, University of Bath.

Rebecca Nonoo from the Department of Chemistry, Imperial College, winner of the poster presentation prize at the symposium, being presented with her cheque for £100 by Professor Barry Potter from the School of Pharmacy, University of Bath.

THE MEDICINAL CHEMISTRY DIVISIONS OF THE TWO BELGIAN CHEMICAL SOCIETIES, "KONINKLIJKE VLAAMSE CHEMISCHE VERENIGING (KVCV)" AND "SOCIÉTÉ ROYALE DE CHIMIE (SRC)"

Emerging Targets and Treatments: Opportunities and Challenges for Drug Design. Annual One-Day Meeting on Medicinal Chemistry of SRC & KVCV
Het Pand, Ghent
November 25, 2011
Website: www.medchem.be
Contact: LD Organisation Scientific Conference Producers
Mail: secretariat@ldorganisation.com

The Medicinal Chemistry Divisions of the two Belgian Chemical Societies, "Koninklijke Vlaamse Chemische Vereniging (KVCV)" and "Société Royale de Chimie (SRC)" are organizing every year an international one day symposium in Belgium, with the aim to update interested participants on selected areas of pharmaceutical research by specialists in their respective field.
In recent years, this symposium has been focusing on topics such as "Does size matter? Beyond small molecule therapeutics: challenges and success stories" (2009), "Small molecules, Antibodies and Natural Products: Multiple Faces of Medicinal Chemistry" (2008); "New Drugs and Drug Candidates: Recent Achievements in Medicinal Chemistry (2007)"; "Personalized Medicine: New Opportunities for Drug Discovery (2006)", or "Targeting the Brain: Successes and Pitfalls (2005)", and has been gathering every year around 170 to 200 participants, half from universities, half from industry, both from Belgium and surrounding countries.

This year's symposium with six invited lectures and three oral communications is scheduled to be held on Friday November 25, 2011, at the conference centre "Het Pand" in Ghent and will be chaired by Prof. Serge Van Calenbergh (UGent). The title and focus of the symposium will be "Emerging Targets and Treatments: Opportunities and Challenges for Drug Design".

Confirmed Speakers to date:

Translocator protein as a promising target for novel anxiolytics
Prof. Federico DA SETTIMO
Università di Pisa, Pisa, Italy

Drug to Genome to Drug: Discovery of New Antiplasmodial Compounds
Prof. Benoit DEPREZ
Université de Lille 2, Lille, France

Selective Androgen Modulators (SARM) for the Treatment of Cachexia
Mr. Pierre DEPREZ
Galapagos, Romainville, France

Therapeutic Targeting of Toll-like Receptors
Dr. Brian KEOGH
Opsona Therapeutics Ltd, Dublin, Ireland

Targeting GSK-3 with ATP Non-Competitive Inhibitors: From the Bench to the Clinical Trials
Prof. Ana MARTINEZ
Instituto de Quimica Medica-Csic, Madrid, Spain

New targets for the treatment of HIV
Dr. David PRYDE
Pfizer Global R&D, Sandwich, United Kingdom

DIVISION OF MEDICINAL CHEMISTRY OF THE SWISS CHEMICAL SOCIETY

News on planned activities 2011 and 2012

Division of Medicinal Chemistry, oral and poster session at the Fall Meeting of the Swiss Chemical Society
EPFL, Lausanne**,** September 9, 2011

Division of Medicinal Chemistry, oral and poster session at the Fall Meeting of the Swiss Chemical Society
ETH Zürich, Zürich, September 13, 2012

A half-day mini-symposium at the University of Basel in May 2012. (the exact date and topic of the event will be announced).

MEDCHEM GROUP OF THE PORTUGUESE CHEMICAL SOCIETY

News on planned activities 2011 and 2012

"1st Fall School on Medicinal Chemistry",
Fátima, Portugal
November 20-23, 2011
The Medicinal Chemistry Group of the Portuguese Chemical Society will run the first Fall School on Medicinal Chemistry ever held in Portugal, to celebrate the UN International Year of Chemistry 2011. It will cover a range of key topics in drug discovery and translational research related to cancer and neurodegenerative diseases and targets scientists from academia and pharmaceutical industry, as well as Ph.D. students.

Third National Meeting on Medicinal Chemistry (ENQT3)
Aveiro University, Portugal.
November, 2012
The third edition of the now traditional National Meeting on Medicinal Chemistry will take place in the University of Aveiro.

EFMC Short Course

4th Short Course on Medicinal Chemistry

SAFETY AND ATTRITION WORKSHOP

December 7-9, 2011

Organisers
Alan Stobie, *Pfizer*
Henk Timmerman, *VU Amsterdam*

Deadline for registration
October 24,2011

Venue
Castle "Oud Poelgeest", Oegstgeest (near Leiden), The Netherlands
Airport: Schiphol (Amsterdam)

Fee
€ 1275,00
Including 3 nights accommodation, breakfast, coffee breaks, lunches and dinners during the 3 days of the conference.

This intensive course is intended for scientists working in the field, and the presentations will be given by senior scientists both from industry and academia. The number of participants will be limited to 35, to favour in depth discussion.

Course Outline
The 4th EFMC Short Course on "Safety and Attrition" will be a repetition of the 2nd Short Course, organised in April 2010.

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EUROPEAN FEDERATION FOR MEDICINAL CHEMISTRY

EFMC | ISMC 2012

XXIInd International Symposium on Medicinal Chemistry

September 2-6, 2012 Berlin, Germany

Mark the dates!

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GDCh Gesellschaft Deutscher Chemiker

DPhG Deutsche Pharmazeutische Gesellschaft e.V.

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PLENARY LECTURES

4 INVITED PLENARY LECTURES
3 EFMC AWARD LECTURES
– The Nauta Award for Pharmacochemistry
– The UCB-Erlich Award for Excellence in Medicinal Chemistry
– The Prous Institute-Overton and Meyer Award for New Technologies in Drug Discovery
2 EFMC PRIZE LECTURES
– Prize for Young Medicinal Chemist in Industry
– Prize for Young Medicinal Chemist in Academia

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