The official EFMC e-newsletter

MedChem Watch

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EFMC

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The European Federation for Medicinal Chemistry (EFMC) is an independent association founded in 1970 that represents 25 scientific organisations from 23 European countries. 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 deepen contacts and exchanges between medicinal chemists in Europe and around the World. EFMC fulfils this objective by organizing symposia and short courses, by sponsoring meetings and medicinal chemistry schools, by publishing on relevant topics and by conferring awards and prizes.

EDITORIAL

Dear colleagues,

In this first issue of the year 2012, it is my pleasure to introduce to all our members the new President of the EFMC, Uli Stilz. After one year of acquaintance as President Elect, Uli acts in is full responsibility starting from January. As it is becoming a tradition for us, we offer to the new President the stage of *MedChemWatch* to presents his program and his vision for the forthcoming years of medicinal chemistry in Europe in an Interview which you find in the next pages.
For a new president there is also a past president. I am sure to interpret the feeling of all of us not only by welcoming Uli in his new position, but also by warningly thanking Gerhard Ecker for what he has done in many years of service for the European Federation. Gerhard has been member and Secretary of the Executive Committee of the EFMC before becoming President for the 2009-2011 term. He was also actively present in the functioning of committees, and lastly but importantly, he was the founder and the first editor of this newsletter. Gerhard will sit again in the EC as Past President, and I am sure he will be a strong resource for our community in the future. Also as demonstration that that active involvement in learned societies can be conjugated with excellent science, we publish here, in this issue, a Lab Presentation of the Gerhard's research group.
This issue of *MedChemWatch* also contains the usual columns. You will find the presentation of the The Organic Chemistry and Natural Products Research Group at Aveiro University, Portugal, and two SME presentation. The first one is from Giuseppe Giardina, who introduce us with NiKem Research (Milan, Italy). The second one is from Cyclofluidic, a UK-based company presented by Elizabeth Farrant.

Finally, please keep in mind that this is an even year, and the ISMC will be the key event. The 22nd EFMC-ISMC will take place in Berlin, September 2-6. The preliminary program is already on line. Don't miss the opportunity to attend to world's largest meeting in medicinal chemistry!

Gabriele Costantino, *Editor of MedChemWatch*

Interview with Dr. Uli Stilz, the New President of EFMC

GABRIELE COSTANTINO

GABRIELE COSTANTINO: Uli, the starting of a new presidency is a good occasion to take stock of the state of EFMC and of medicinal chemistry in general in Europe. What's your vision for the next years?

ULI STILZ: Gabriele, let me first of all express that it is a special honor for me and makes me feel privileged to have been elected by the Council as President of the EFMC from 2012 to 2014. The year 2011 has been a year of continued economic crisis and of unprecedented change for many of our members in the pharmaceutical industry. Across the board R&D activities have been challenged in view of continuously rising R&D costs for each NCE or NBE being approved and pressures from business to maintain profitability in view of a significant patent cliff and cost pressures in global health care systems. At the same time we are experiencing remarkable scientific advances as a community moving us towards a better understanding of human disease biology. Overall I believe that we will need to take more risk in research to push for disruptive innovation over incremental improvements. Chemists will have to play a key role here to advance our molecular understanding of disease, to study complex systems, and to make sophisticated molecules. Medicinal Chemistry has always been an interdisciplinary field with the ability to make molecules – either small or large – at its core. We certainly need to foster the science of making and improving drug like molecules and we need to train young scientists in the art of doing so. At the same time I would like us, the chemical community, to be engaged in current and future frontiers including pathway biology and target selection, translational science and biomarker discovery, and disruptive drug targeting and delivery solutions. All this will require new ways of working across various disciplines both in academia and industry. Activities of the EFMC in the coming years are intended to both foster the scientific excellence and training of our discipline in Europe and at the same time to facilitate collaborations across scientific disciplines including biology and medicine. I see the role of the EFMC in shaping this interdisciplinary research environment and in promoting Medicinal Chemistry across Europe using the large research network we already have. We can build hereby on the enthusiasm and scientific reputation of our scientific community and on the legacy and vision of EFMC's past presidents Henk Timmerman, Ferran Sanz, Roberto Pellicciari, and Gerhard Ecker.

GC: Can you anticipate your main commitments as President of the EFMC? What will be the continuities with the former presidencies, and what the innovation you intend to bring up?

US: EFMC today is a very well organized learned society with a well established infrastructure supporting our activities. It is one of my commitments to seek an active dialog with the scientific and strategic committees of the EFMC to jointly shape our strategic vision and operational activities. It is also critical that we maintain our infrastructure and secure the required finances to do so. We certainly will continue to foster scientific networks across the globe. Our scientific meetings including EFMC-ISMC provide a wonderful platform for this. It is important for me that we also continue to invest into the future of young scientists by providing

training opportunities including short courses and travel grants.
Looking into the future I would like EFMC leadership to actively engage in a dialogue with their members and to build opportunities for member scientists to network with each other. The social media provide us here with a unique opportunity and we will need to figure out how to best navigate in this space.
In addition, I would like us to be active participants in the European Biomedical Science community. It is important that we expand our networks further into the basic disease biology as well as the medical/clinical communities as I believe that innovation will be driven at these interfaces. Furthermore it is one of my and the EC's priorities to leverage EFMC member's knowledge to influence European science policies. We have been actively involved in the Innovative Medicine Initiative and I expect future initiatives to involve Medicinal Chemistry even more closely as an enabling science.

GC: EFMC gathers together more than 6,000 medicinal chemists from both academia and industry. European medicinal chemistry has the potential for being one of the world-leading drivers of the research in biochemical and health sciences. What are your personal and the EFMC's commitments to create a real community of medicinal chemists in Europe, from both a cultural, political and economical point of view?

US: Today Medicinal Chemistry in Europe is well networked across the various member states.
The EFMC-ISMC is the World's largest medicinal chemistry meeting, bringing together more than 1000 scientists every other year to discuss most scientific advances and new clinical candidates.
We also foster a significant number of national and international meetings and training events mentioned below in more detail. This emphasizes that we already have a dynamic and innovative scientific community driving biomedical innovation and drug discovery.
We are collaborating with other learned societies both in and outside Europe. I just would like to mention our participation in the European Pharma Leadership forum which gives us the opportunity to discuss and share our vision with other learned societies in Europe and to influence science policies in Europe. It goes without saying for all of us that novel medicines will be molecular entities but nevertheless we should not get tired to communicate that the ability to design and synthesize new molecules – small molecules or macromolecules – will be a critical enabler of any biomedical research enterprise.

GC: One of the missions of EFMC is to promote aggregation and cultural exchange between the members. Can you briefly summarize what are the main activities of EFMC, and which instruments can an European medicinal chemist use to get information about EFMC and its activities (besides this newsletter, of course)?

US: Scientific meetings will continue to be critical activities to bring the medicinal chemistry community together to learn about the newest science and to network amongst scientists. Our flagship event is the biannual EFMC-ISMC meeting which will be held in Berlin in 2012 and in Lisbon in 2014. In addition, we organize the ASMC together with Chembridge and the Frontiers in Medicinal Chemistry series together with ACS every other year. We also sponsor a significant number of scientific events of our member societies each year.
Education and Training is a cornerstone of the mission of EFMC and is provided to young scientists and industrial researchers through our summer schools and short courses.
Among them, I would like to highlight the Medicinal Chemistry Schools. Besides the accredited Summer School in Urbino (Italy) the EFMC sponsors additional 5 summer schools.
Short courses are intended for scientists working in the field, and the presentations are given by senior scientists from both industry and academia. The number of participants is limited to 35 to allow for in depth discussions.
The next course in 2012 (April 1-4) will be organized by Thomas Klabunde (Sanofi), Brian Harms (Merrimack), and Henk Timmerman (Amsterdam) and will be focused on the topic "Target selection through chemical and systems biology". The Fall Short Course is scheduled for October 21-24, 2012. Topic will be "Improving Compound Quality: Physical Chemistry and DMPK Properties in Drug Discovery. Principles, Assays and Predictions" and the programme will be compiled by Kevin Beaumont (Pfizer).
Each year we publish our yearbook Medicinal Chemistry in Europe. In 2012 we have moved from the previous print version only to a mixed model with an electronic version complemented by printed versions on request to account for the growing number of our members preferring to use electronic media. Finally, we have MedChemWatch, the e-newsletter of EFMC, which is

also incorporated into the paper version of MedChemComm, our monthly journal published by RSC containing a mix of vibrant and concise research and review articles. Thinking about electronic media we have created an expert network within LinkedIn more recently. I believe that social media offer a significant opportunity to create a lively and interactive community and right now we are looking into various options on how to best navigate and on how to best involve our members to make this happen.
We also convene three major EFMC awards each second year, we established the EFMC Prize for a Young Medicinal Chemist in Industry and the EFMC Prize for a Young Medicinal Chemist in Academia and we have session exchange agreements with three major international learned societies.
If you would like to obtain up to date information on EFMC activities please register on our web page www.efmc.info.

GC: Thank you very much and good luck for your presidency ! Would you like to conclude by addressing a short message to all the readers of this newsletter?

US: Yes, certainly. I would like to encourage you all to actively participate in the community and shape Medicinal Chemistry in Europe with your ideas and your enthusiasm. Please don't hesitate to reach out to me with your ideas, wishes, and concerns.

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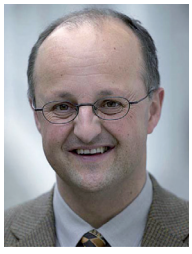


Uli Stilz did his undergraduate training at the University of Freiburg and the ETH Zuerich culminating with a Master degree in Organic Chemistry. He then moved to the Max-Planck-Institute in Martinsried, where he received his Ph.D. in Biochemistry in 1990. Subsequently, he undertook post-doctorial studies at the California Institute of Technology.
In 1992 he joined Hoechst AG in Frankfurt as Research Scientist working initially on cell adhesion inhibitors. In 1997 he was appointed Research Director in Medicinal Chemistry. As of 1999 he became responsible for Discovery Chemistry at the Frankfurt Research Site. Under his leadership, the team delivered multiple candidates now under clinical evaluation at various stages. In 2007 he was appointed Associate Vice President in Chemical and Analytical Sciences with responsibility for research groups in France, Germany, and the United States. As of 2010 he has assumed responsibility for the innovation department within the Diabetes Division with a special emphasis on disease biology, regenerative medicine, systems biology/bioinformatics, diagnostics/biomarkers, and innovative devices.
He is president of the European Federation for Medicinal Chemistry and serves on various Editorial and Scientific Advisory Boards.

The Pharmacoinformatics Research Group
University of Vienna

GERHARD F. ECKER

The Pharmacoinformatics Research Group

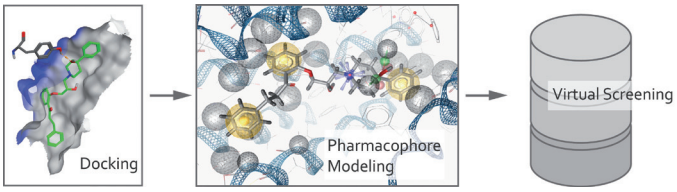
Originally established as Emerging Field Pharmacoinformatics at the Faculty of Life Sciences at the University of Vienna, the Emerging Field developed towards a full professorship of Pharmacoinformatics.

The international team, headed by Prof. Dr. Gerhard Ecker, follows a holistic approach, combining multi-dimensional annotation, structural modeling of biomolecular systems, structure-based drug design, chemometric and in silico chemogenomic methods, statistical modeling and machine learning approaches, to develop predictive computational models. The experimental validation and optimisation of the obtained *in silico* models by strong links to experimental groups is an integral part of these activities. Currently the targets under investigation include several ABC-transporter (ABCB1, ABCC2, ABCB11, ABCG2), the serotonin and dopamine transporter, the GABA transporters, the hERG potassium channel, the TRPV1 channel, the $GABA_A$ receptor, and the insulin receptor. On a methodological basis, the group works on development of new, similarity-based descriptors and the application of unsupervised neural networks for hit-identification.

Ligand-based Studies on ABC-transporters

The main line of research is along the molecular basis of drug-transporter interaction. This started in 1993 with the discovery that the class 1C antiarrhythmic agent propafenone is able to inhibit the multidrug transporter P-glycoprotein (P-gp, ABCB1). P-gp transports a wide variety of functionally and structurally diverse cytostatic agents out of tumor cells, thus preventing accumulation of these drugs within the cells. Inhibition of the transport leads to resensitisation of multidrug resistant cells and thus presents a useful concept for therapy of resistant tumors. Analogous transport systems were also identified in bacteria and fungi. In a strong collaboration with Peter Chiba from the Medical University of Vienna we started a lead optimization program using mainly 2D- and 3D-QSAR studies, which resulted in several tool compounds with potency in the nanomolar range. Besides standard techniques such as Hansch-analysis, Free-Wilson analysis, CoMFA, and GRIND, the group also explores the potential of artificial neural networks, i.e. feedforward backpropagation networks and self organizing maps. The latter have also been successfully applied for scaffold hopping and virtual screening, both for identification of new P-gp inhibitors and insulin receptor activators, as well as for classification of hERG channel blockers.

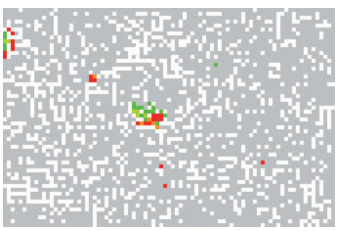
P-glycoprotein and related transporters are also strongly influencing ADME properties, such as intestinal absorption, blood-brain barrier permeation, and canalicular excretion. Thus, substrates of P-gp and related transporters might face the risk of poor bioavailability, while inhibitors may lead to drug/drug interactions and drug induced cholestasis. The group is thus also actively engaged in developing classification models for prediction of P-gp substrates and inhibitors. In order to mimic real life scenarios, where the number of inactives by far exceeds the number of actives (100:1 to 1000:1), machine learning methods such as random forest and support vector machines, both combined with cost sensitive bagging, are applied for classification of large data sets.



The application of a SAR-guided docking protocol provided a highly reliable binding hypothesis for a class of P-gp inhibitors. Out of this binding mode a structure based pharmacophore model was generated, which in turn was used for virtually screening commercial vendor databases for identifying new P-gp inhibitors.

Experimental Data Guided Ligand Docking

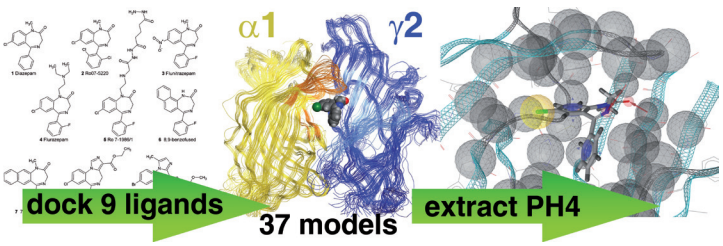
One major focus of the Pharmacoinformatics Research Group is to combine ligand- and structure-based methods. Briefly, the extensive ligand-based in silico studies reveal a clear picture on pharmacophoric sub structures and guide the selection of compounds to be docked into protein homology models of the target under consideration. Subsequent unrestrained docking of these ligands followed by clustering of common scaffolds reveals clusters of binding hypotheses, which are prioritized and validated on basis of the SAR known. As a final prove of concept, top prioritized poses serve as basis for the generation of structure-based pharmacophore models, which are used for screening vendor libraries. Top ranked compounds are ordered and biologically tested. This approach has been successfully applied for identification of new ligands of the benzodiazepine binding site at the GABA-A receptor, inhibitors of P-gp, and inhibitors of the serotonin transporter. The latter two projects are pursued under the framework of the national research cluster SFB35 – "Transmembrane Transporters in Health and Disease" (www.sfb35.at).



Self-organizing maps as screening tools: Compounds with known activity (green: active, red: inactive) are trained with compounds from a screening database (grey) to find new hits.

Current and Future Challenges

With the increased understanding of physiological and pathophysiological processes driven by systems biology, pharmacoinformatics will move towards pathway driven drug discovery and integrated approaches. First attempts made in our group focus on prediction of cns related side effects of antidepressant agents based on their interaction profiles with a set of 30 transporters and receptors expressed in the cns. Another challenge, the prediction of the outcome of a 28 day rat toxicity study, is pursued under the framework of eTOX, a European project funded by the Innovative Medicines Initative (IMI; www.imi.europa.eu). Finally, by coordinating the Open PHACTS project (www.openphacts.org), the group made a strong move towards semantic integration of public and private data sources relevant for drug discovery. Open PHACTS is also funded by the IMI and aims at developing an Open Pharmacological Space utilising sematic web technology based on rdf triples and nanopublications. This will allow to answer questions such as "*give me all compounds which have been annotated with liver toxicity and the interaction profile of these compounds with all transporters expressed in the liver*" within a few minutes.



In the search for the binding mode of diazepam at the GABAA-receptor we conducted an exhaustive docking run. We docked a total of nine 5-aryl-1,4-benzodiazepines into 37 homology models of the benzodiazepine binding site of the GABAA receptor, considering flexible side-chains. We retained the 100 best scored poses per docking run. The huge amount of poses was then clustered according to their common 1,4-benzodiazepine scaffold. Following the hypothesis that similar ligands bind in a similar manner, we rejected clusters that could not accommodate essential ligands. The three remaining clusters were heavily evaluated against experimental data resulting in one clear favorite cluster, representing the proposed binding mode. Finally a structure-based pharmacophore was extracted from this final binding mode. This model was then used in a virtual screening study, leading to the identification of a new, experimentally validated, benzodiazepine binding site ligand.

About Gerhard Ecker

Gerhard Ecker is Professor for Pharmacoinformatics and Head of the Pharmacoinformatics Research Group at the Department of Medicinal Chemistry, University of Vienna. He also coordinates the research focus "Computational Life Sciences" of the Faculty of Life Sciences. Gerhard received his doctorate in natural sciences from the University of Vienna and performed his post-doctoral training at the group of J. Seydel in Borstel (Germany). He has published more than 100 articles mainly related to SAR and QSAR studies on P-glycoprotein (P-gp), edited 3 books and gave more than 100 invited lectures. Gerhard is Editor of Molecular Informatics and member of Editorial Advisory Boards and Editorial Boards of several journals. In the years 2009 – 2011 he served as President of the European Federation for Medicinal Chemistry (EFMC), and from 2012 on he chairs the Strategic Advisory Board of EFMC. Finally, he is also strongly engaged in national and international educational activities, such as the national PhD network "Molecular drug targets" (moltag.univie.ac.at) and the EUROPIN PhD Programme in Pharmacoinformatics (www.europin.at), which comprises seven top groups in the field of pharmacoinformatics from 6 European countries.

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The Organic Chemistry and Natural Products Research Group

Aveiro University

JOSÉ CAVALEIRO, ARTUR SILVA

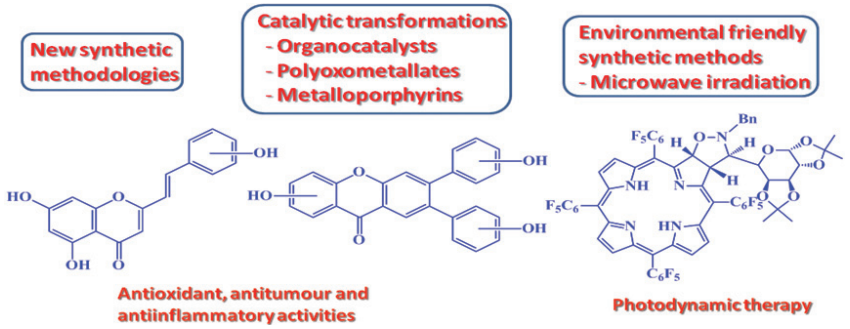
The Aveiro *Organic Chemistry and Natural Products Group* is performing its research activities in the Department of Chemistry of the local University. Such activities are centered on the development of new synthetic methodologies leading to biologically significant new products. The latter include tetrapyrrolic macrocycles and of some of their metal complexes, polyphenolic compounds, quinolone and acridone derivatives, and cyclohexane derivatives bearing several stereocenters. Regio- and enantioselective organocatalytic conjugated additions, diastereoselective domino multicomponent reactions, homogeneous and heterogeneous catalytic transformations, using polyoxotungstates and metalloporphyrins as catalysts, and the use of microwave irradiation in the chemical transformations under study are also targets in the mentioned studies. In interdisciplinary approaches and looking for potential applications concerned with the valorisation of the new compounds, the following working lines are considered: i) use of porphyrin derivatives, as photosensitizers, in cancer treatment and in the photoinactivation of microorganisms; ii) use of nitrogen and oxygen heterocyclic compounds as anti-inflammatory and antitumour agents and as food additives.

Prof. José Cavaleiro was the founder of this research group in the University of Aveiro and is full professor of Organic Chemistry since 1986. He is the main responsible for the tetrapyrrolic macrocycles research line. Prof. Artur Silva was a student at the University of Aveiro, PhD student of Prof. José Cavaleiro and is full professor of Organic Chemistry since 2001. He is the main responsible for the nitrogen and oxygen heterocyclic (mainly polyphenols) compounds research line. Both research lines are also interested in the catalytic transformations, using organocatalysts or polyoxotungstates and metalloporphyrins as catalysts.

In the last decade, we have a long track in the development of new synthetic methods for several polyphenolic compounds (*e.g.* 2- and 3-styrylchromones, xanthones, flavones) and in the preparation of several new derivatives to be assessed as antioxidant and anti-inflammatory agents. These studies showed that polyhydroxy-2-styrylchromones exhibited potent xanthine oxidase inhibitory activity, protective effects against the hepatotoxicity mediated by pro-oxidant agents, and important antioxidant properties. We also demonstrated that active antioxidant 2-styrylchromones are also potent inhibitors of LOX and COX enzymes. It was also demonstrated that polyhydroxy-2,3-diarylxanthones present an outstanding ROS and RNS scavenging properties, considering the nanomolar to micromolar range of the IC50 values found. The xanthones with two catechol rings were the most potent scavengers of all tested ROS and RNS. These antioxidants are also superior to quercetin in protecting human skin keratinocytes against *tert*-butylhydroperoxide induced oxidative stress and also in the inhibition of Cu^{2+}-induced lipid peroxidation of human LDL.

The transformation of some of the referred polyphenolic compounds throughout cycloaddition and cross-coupling reactions and also the establishment of new synthetic methods of nitrogen heterocyclic compounds, such as pyrazoles, triazoles, acridones and 4-quinolones, due to their potential important biological activities, have also been one of our main target of work.

The design of complex organic molecules with multiple stereogenic centres is a continuing challenge at the forefront of



synthetic chemistry. One approach to this challenge involves the development of catalytic domino, cascade or tandem multicomponent reactions. For a long time, asymmetric organocatalysis, in which small chiral organic molecules act as active species, was predominated in the field of organic synthesis because are metal free, usually nontoxic and environmentally friendly. Recently, we have also developed novel diastereoselective domino multicomponent reactions under phase-transfer conditions to construct cyclohexane derivatives with five new stereocenters, which contain hydroxy, nitro and ketone functional groups and a quaternary carbon atom. Structures that include a stereogenic quaternary carbon are one of the most demanding topics in the synthesis of natural products and pharmaceutical agents.

During the last two decades, porphyrins, corroles and phthalocyanines are being explored as important tools for new applications, such as catalysts, advanced biomimetic models for photosynthesis, new electronic materials, sensors and as drugs. We have been focused on the synthesis and transformation of tetrapyrrolic macrocycles into new derivatives with improved features that may turn them possible candidates to be used in different areas. These studies included: i) functionalization of porphyrins and corroles through cycloaddition reactions, reactions involving transition metal catalysts and nucleophilic aromatic substitution; ii) development of new porphyrin derivatives and analogues with adequate structural characteristics to be used as photosensitizers in PDT, to be evaluated for their bactericidal, fungicidal, virucidal and antitumoral activities; iii) preparation and characterization of novel homogeneous and heterogeneous catalysts based on iron or manganese substituted polyoxotungstates and metalloporphyrins and analogues, including the evaluation of their catalytic performance in the oxidation of aromatic hydrocarbons, aromatic heterocycles and terpenes; iv) preparation of phthalocyanines and calix[4] pyrrole derivatives and their use as anion sensors.

Our synthetic work aims to establish novel synthetic methods, using environmental friendly synthetic approaches, so we have been developing new methods using microwave irradiation as the energy source, in solvent free-conditions or under a reduced volume of organic solvents.

These pioneering studies on polyphenolic compounds and tetrapyrrolic macrocycles demonstrate that new bioactive agents with a desired structural profile can be obtained.

2-Styrylchromones an useful synthetic synthon and a source of potential drugs

The inflammatory process is a complex physiological response, which involves an increase in vascular permeability as well as release of lipid-derived autacoids, but also an overproduction of reactive oxygen and nitrogen species (ROS and RNS). If these reactive species overcome host defense systems, exacerbated damage in inflammatory sites may occurred, contributing to chronic diseases. Therefore, in order to control these diseases, anti-inflammatory substances need to be used that should also possess antioxidant properties. Polyphenolic compounds have drawn a great deal of attention compared to other natural products mainly due to their antioxidant, anti-inflammatory and anticarcinogenic properties. The similarity of 2-styrylchromones with flavones and some of their know biological activity led us to develop new synthetic methods for this type of compounds and to design some novel molecules which have present important antioxidant, anti-inflammatory, and anti-norovirus activities while a certain derivatives was identified as a selective proliferation inhibitor of human tumor (MCF-7 and NCI-H460) cell lines.

2-Styrylchromones were also the starting material, throughout cross-coupling reactions, for the development of a novel group of polyphenolic compounds, polyhydroxy-2,3-diarylxanthones, for which we have also already demonstrated potent antioxidant activities. Some of the biological applications of these compounds were the subject of a European patent application.

All this *trans*-disciplinary work was developed in collaboration with some Portuguese (*Eduarda Fernandes and M. São José Nascimento, Pharmacy Faculty of Porto*) and French (*René Santus, Muséum National d'Histoire Naturelle de Paris, and Patrice Morliére, Laboratoire de Biochimie, CHU Amiens*) research groups.

Cationic and glycoconjugate porphyrin derivatives

Structural features are required for a new porphyrin derivative to be considered as a photosensitizer (PS) in photodynamic therapy (PDT). And for that each new PS must exhibit adequate amphiphilic properties. And these have been big synthetic challenges. In such way dihydro-type or tetrahydro-type porphyrins (respectively chlorins and bacteriochlorins) as well as certain cationic and glycoconjugate derivatives have been targets for several research groups.

We have been able to establish that certain porphyrin macrocycles can act as dienophiles or dipolarophiles in Diels-Alder cycloadditions; in such way novel chlorin or bacteriochlorin types can become available. The formation of glycoconjugates can also be obtained in such way. It was also demonstrated that novel cationic derivatives can become available by using our reported methodology. In collaboration with other groups the new products have been assessed as photosensitizing agents in PDT or in the photoinactivation of microorganisms. In particular the action against antibiotic resistant bacteria, mainly the Gram (-) ones, is of great significance. It is also possible to photoinactivate microorganisms present in water samples, including sewage ones. Such potential applications have been patented.

The biological assesssment work has been carried out in collaboration with colleagues from other areas (Biology departments of the Universities of Aveiro, Lisbon, Padova, Humboldt, Autonoma-Madrid and from Muséum National d'Histoire Naturelle de Paris, and Laboratoire de Biochimie, CHU Amiens).

Contact

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web: http://www.ua.pt/dq/PageText.aspx?id=6340

Selected recent publications

1 Carvalho C. M. B. , Neves M. G. P. M. S., Tomé A. C., Paz F. A. A., Silva A. M. S., Cavaleiro J. A. S., 1,3-Dioxopyrrolo[3,4-b]porphyrins: Synthesis and Chemistry, *Org. Lett.*, **2011,** 13, 130-133.

2 Santos C. M. M., Freitas M., Ribeiro D., Gomes A., Silva A. M. S., Cavaleiro J. A. S., Fernandes E., 2,3-Diarylxanthones as strong scavengers of reactive oxygen and nitrogen species: A structure-activity relationship study, *Bioorg. Med. Chem.*, **2010,** 18, 6776-6784.

3 Pereira A. M. V. M., Neves M. G. P. M. S., Cavaleiro J. A. S., Jeandon C., Gisselbrecht J.-P., Choua S., Ruppert R., Diporphyrinylamines: Synthesis and Electrochemistry, *Org. Lett.,* **2011,** 13, 4742-4745.

4 Carvalho C., Alves E.,Costa L. , Tomé J. P. C., Faustino M. A. F., Neves M. G. P. M. S., Tomé A. C., Cavaleiro J. A. S., Almeida Â., Cunha Â., Lin Z.,Rocha J., Functional Cationic Nanomagnet-Porphyrin Hybrids for the Photoinactivation of Microorganisms, *ACS Nano*, **2010,** 4, 7133-7140.

5 Oliva C. G., Silva A. M. S., Paz F. A. A., Cavaleiro J. A. S., Highly Enantioselective and Regioselective Conjugate Addition of Nitromethane top 1,5-Diarylpenta-2,4-dien-1-ones Using Bifunctionla Cinchona Organocatalysts, *Synlett,* **2010,** 1123-1127.

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9 Alves E., Faustino M. A. F., Tomé J. P. C., Neves M. G. P. M. S., Tomé A. C., Cavaleiro J. A. S., A. Cunha, Gomes N. C. M., Almeida A., Photodynamic Antimicrobial Chemotherapy in Aquaculture: Photoinactivation Studies of Vibrio fischeri, *PloS One,* **2011,** 6, e20970-e20978.

10 Almeida A. I. S., Silva A. M. S., Cavaleiro J. A. S., Reactivity of 3-Iodo-4-quinolones in Heck Reactions: Synthesis of Novel (E)-3-Styryl-4-quinolones, *Synlett,* **2010,** 462-466.

11 Santos C. M. M., Silva A. M. S., Filipe P., Santus R., Patterson L. K., Mazière J.-C., Cavaleiro J. A. S., Morlière P., Structure-activity relationship in hydroxy-2,3-diarylxanthone antioxidants. Fast kinetic spectroscopy as
12 a tool to evaluate the potential for antioxidant activity in biological systems, *Org. Biomol. Chem.,* **2011,** 9, 3965-3974.

13 Gomes A. T. P. C., Cunha A. C., Domingues M. R. M., Neves M. G. P. M. S., Tomé A. C., Silva A. M. S., Santos F. C., Souza M. C. B. V., Ferreira V. F., Cavaleiro J. A. S., Synthesis and characterization of new porphyrin/4-quinolone conjugates",*Tetrahedron,* **2011,** 67, 7336-7342.

NiKem Research Srl

GIUSEPPE GIARDINA*

NiKem Research Srl (NiKem) started operations in 2001 as a spin-off from the SmithKline Beecham (GSK) Milan Discovery centre and is located at Baranzate (Mi, Italy); it is a specialized drug discovery company whose mission is to create value to the Pharmaceutical Industry capitalizing on the over 20-year average experience in medicinal chemistry and drug discovery cumulated by its Management Team within a multinational company.

NiKem has an international reputation as a strategic and consolidated partner on the basis of more than ten years of operations in Pharmaceutical Research and Development offering a wide range of services, such as synthetic and medicinal chemistry, biochemical pharmacology, *in vitro* ADMET, *in vivo* DMPK and preliminary rodent toxicology, preclinical GLP and clinical GCP bioanalysis. All these modules can be sold as an integrated platform or as standalone services, thus allowing great flexibility to the business model and great compliance with client's needs.

To fully realize its value proposition, NiKem implemented and developed an appropriate infrastructure in terms of facilities, technology platform and equipments, all instrumental to offer a demonstrated advantage to its clients. Making the best use of this technology platform, NiKem scientists are able to offer an added value output obtained in the shortest possible timeframe with a significant return on investment for the outsourcing company.

The hidden gem inside NiKem is actually its staff, a balanced mix of synthetic and medicinal chemists, biologists and biotechnologists, most of them with more than 10 years of experience in the pharmaceutical sector, very well coordinated and supervised by the Management Team with over 25 years in average of experience in drug discovery. In view of the increased competition in the outsourcing drug discovery arena, it is not enough to have well trained people and best scientific competence and technologies. NiKem is fully oriented to understand and satisfy the different needs of its clients, implementing customer-tailored solutions and adopting a client-oriented flexibility. This means that NiKem not only has a well trained and experienced staff but also that these people are able to work together in a "team approach model". Given the multidisciplinary environment of the drug discovery & development process this is a great plus as NiKem teams perfectly know "when" a certain phase or issue will come during the process and "how" it should be solved.

To boost the competitiveness of the company, at the end of 2007 NiKem implemented a 3-year strategic industrial development plan to integrate the technologies and skills already existing on site with new emerging technologies and certifications:

– MALDI/TOF/TOF (Mass Spectrometry time of flight) for ex vivo 'imaging' studies;

– Expansion of services within rodents in vivo treatments (pharmacokinetics, toxicokinetics, PK/PD, and in vivo pharmacology);

– Achievement of Good Laboratory Practice (GLP) certification for pharmacokinetic and metabolism (Cer-

tificate of Compliance to the Good Laboratory Practice, granted from the Ministry of Health in 2009);

– Achievement of authorization to perform rodent acute and sub-chronic toxicology and toxicokinetic studies (Authorization by Ministry of Health Decree in 2010);

– Achievement of qualification and subsequent authorization in 2010-2011 from regulatory authorities (AIFA – Italian Agency for Medicines) to perform pharmacokinetic, metabolism and bioequivalence analyses on human samples (plasma, blood, urine, etc.) coming from Phase 1-3 clinical studies.

The excellence of NiKem staff is testified by the 54 patents filed in 11 years (NiKem scientists as inventors and the various clients as assignees) and by the 66 articles published on top international journals on various aspects of medicinal and synthetic chemistry, biochemical pharmacology, pharmacokinetic and drug discovery strategy. From its inception, NiKem has conducted more than 80 medicinal chemistry projects for its clients and more than 100 custom synthesis projects, including 12 library syntheses for either big or mid-size pharmaceutical or small biotechnology companies. Within the medicinal chemistry projects, 11 compounds were approved, by specific Strategic Development Review Board internal to clients' corporate organizations, for progression to full Pre-Clinical Development and 7 of these are today in Clinical Trials (Phase 1 or 2).

***Giuseppe Giardina**
CEO & Managing Director

Contact
NiKem Research
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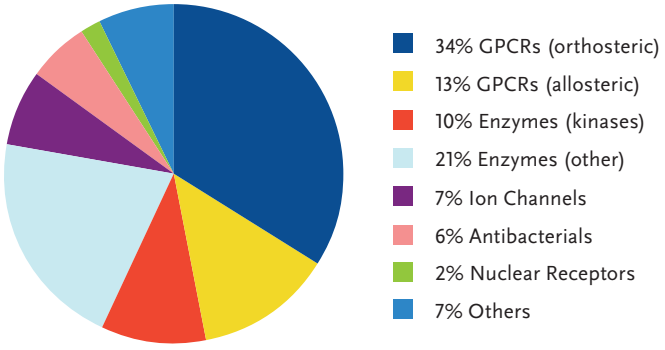
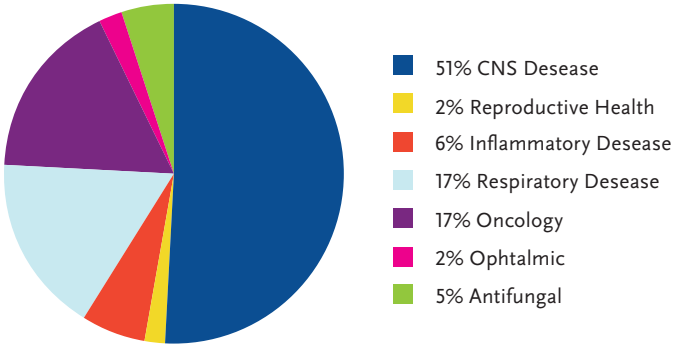
With reference to their mechanism of action, the medicinal chemistry projects can be subdivided as follows:



Project by Mechanism of Action

Instead, with reference to the patents filed by NiKem inventors, the following therapeutic areas of primary unmet medical need, are covered:



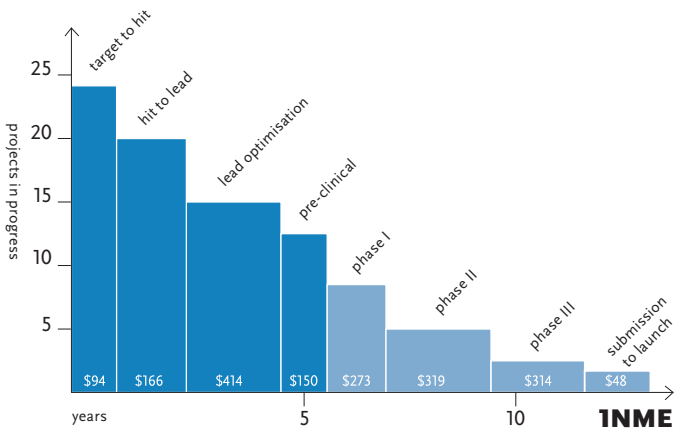
Patents with NiKem Inventors

Cyclofluidic

ELIZABETH FARRANT

Drug Discovery

The process of discovering a drug is slow and expensive, with the average cost of developing a new molecular entity (NME) now estimated at $1.8 billion.



Drug Discovery pipeline to produce 1NME including cost per phase ($M)[1]

Recent analysis has shown that for every NME launched, 19.4 hit to lead programmes are required, at a cost per launch of $166 million, due to the high attrition rates in the drug discovery process. In addition, although much of this attrition (27%) is attributed to lack of efficacy in humans in phase II, the majority is reported to be related to safety, toxicology, formulation, pharmacokinetics and cost of goods (53%). These characteristics are defined by the chemical structure of the molecule itself.

The Importance of Getting the Right Lead Molecule

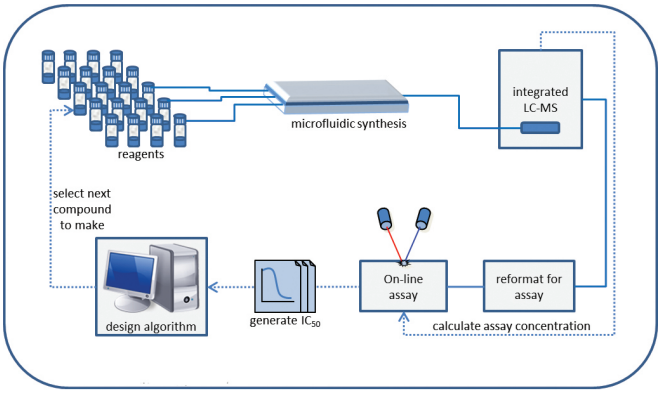
Studies have also shown that drug structures are very closely related to their leads and these leads to the hit series from which they were optimised, indicating that much of the success or failure of a potential drug molecule is laid down at this very early point in the drug discovery process. The decision on which lead series to pursue in the hit to lead phase is therefore crucial and often dictates the quality of the pre-clinical candidate and therefore the success of the programme and the time and resource required to launch.

Medicinal Chemistry

Small molecule lead discovery involves an iterative process of molecular design, chemical synthesis, biological assay and analysis to feed into the next learning cycle. In a typical hit to lead project, in vitro assays are used to measure the potency and selectivity of the molecule at the target of interest as well as a range of calculated and measured physical properties that help to predict a lead molecule's "drug-likeness". Using conventional approaches, each learning cycle in this process takes 1-8 weeks, depending on where compounds are made and tested. These cycle times lead to slow and expensive hit to lead exploration, limiting the number of lead series that can be assessed. In addition, compounds are often designed and made "at risk" i.e. without incorporating the latest data from previous design cycles, leading to wasted effort and resource. This means that lead optimisation can be long and costly and the choice of molecules available to be progressed to pre-clinical studies is sub-optimal.

The Cyclofluidic Approach

The Cyclofluidic technology platform integrates all these processes on the bench-top, allowing drug lead molecules to be assayed minutes (rather than weeks) after they are designed. Potential lead molecules are synthesised, purified and screened in fast serial mode, incorporating activity data from each compound as it is generated before selecting the next compound to make.



The Cyclofluidic Approach

To ensure data quality, each compound is purified by integrated high pressure liquid chromatography (HPLC), its identity confirmed by mass spectrometry and the concentration entering the assay determined in real time by evaporative light scattering detection (ELSD). The compound's IC50 is then measured in an on-line biochemical assay and this result fed into the design selection algorithm before the algorithm selects the next compound to make. The system is designed to use interchangeable design algorithms, assay formats and chemistries and at any stage a medicinal chemist can intervene in order to adjust the design strategy.

About Cyclofluidic

Cyclofluidic has been located in labs in Welwyn Garden City UK since early 2009 after being established as a joint pre-competitive investment between pharmaceutical companies UCB and Pfizer with a collaborative research grant from the UK Government Technology Strategy Board. The company was set up to leverage UK expertise in drug discovery and microfluidic technology in order to develop an integrated automated platform that significantly shortens the design-synthesis-test cycle from weeks to minutes allowing a step change in the ability to discover quality leads. The company is currently working with pharma and academic groups to apply its technology in tool and lead discovery projects.

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EFMC Short Course

6th Short Course on Medicinal Chemistry

IMPROVING COMPOUND QUALITY: PHYSICAL CHEMISTRY AND DMPK PROPERTIES IN DRUG DISCOVERY. PRINCIPLES, ASSAYS AND PREDICTIONS

October 21-24, 2012

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

Course Outline

In modern drug discovery, it is important that the Medicinal Chemist understands how to balance potency and ADME properties in order to provide high quality compounds for progression to clinical studies. This short course will be a mixture of talks and worked exercises designed to further the understanding of DMPK.

The course will include: Outlines of the key DMPK in vitro assays: physicochemistry for ADME; Oral drug absorption; Fundamentals of drug distribution; drug metabolizing enzymes; drug transport proteins; basic PK principles and human PK prediction; PKPD relationships.

Course Organisers
Kevin Beaumont, *Pfizer, USA*
Local Organiser
Henk Timmerman, *VU University Amsterdam, NL*

Deadline for preregistration
September 15, 2012

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

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EUROPEAN FEDERATION FOR MEDICINAL CHEMISTRY

EFMC NEWS

BY NELE COULIER AND KOEN AUGUSTYNS

EFMC is funding grants for EFMC organised events with the aim to support the participation of young academic scientists. Upon application, up to 50% of the registration fee for EFMC-ISMC, EFMC Short Courses or the EFMC Accredited School will be covered by EFMC. To apply for an EFMC grant, please fill in the application form available on the website www.efmc.info before the deadline and upload your CV, publication list, abstract, motivation letter and support letter from the supervisor.

In addition to the EFMC grants, EFMC and the Scientific Committee of ESMEC are offering 13 free registrations for participation at the European School of Medicinal Chemistry (ESMEC) to students from outside Italy. The School, accredited by EFMC, will be held on July 2-7, 2012 in Urbino, Italy. The scholarships, covering the registration fee and the full board accommodation, will be assigned to PhD students enrolled in Doctoral Schools held in one of the member countries of EFMC, excluding Italy. The programme is available on the website www.esmec.eu

To apply for a free registration for ESMEC, please fill in the ESMEC grants application form available on www.efmc.info and send it together with a CV, a motivation letter and an abstract to Prof. Carlo De Micheli (carlo.demicheli@unimi.it) before April 5th. The abstract should summarize the research carried out during the PhD (for abstract instructions, please visit the ESMEC website), and is a prerequisite for the poster that will be presented during the School.

EFMC-ISMC 2012, the 22nd edition of the EFMC International Symposium on Medicinal Chemistry, will take place in Berlin, Germany on September 2-6, 2012. The Symposium, which is internationally recognized as one of the leading Medicinal Chemistry meetings, will provide an international forum for presentations and discussions for leaders in trends in Medicinal Chemistry.

The ISMC symposia traditionally attracts experts in drug discovery and development, in particular medicinal and synthetic chemists, together with scientists active in the fields of computer-assisted drug design, biology, DMPK, pharmacology, early toxicology, as well as chemical and pharmaceutical development. The list of confirmed invited speakers as well as the preliminary programme is now available on the symposium website www.ismc2012.org

Also in 2012, EFMC will organise two EFMC Short Courses on Medicinal Chemistry. The Spring Course, scheduled for April 1-4, 2012, will focus on "Target Selection through Application of Chemical and Systems Biology". The Fall Course will be organised on October 21-24, 2012, focusing on "Improving Compound Quality: Physical Chemistry and DMPK Properties in Drug Discovery. Principles, Assays and Predictions". More information is available on www.efmcshortcourses.org

Join us on LinkedIn!
Become member of the EFMC LinkedIn group and stay updated on EFMC activities.

EFMC EVENTS

BY NELE COULIER AND KOEN AUGUSTYNS

EFMC ORGANISED EVENTS

5th EFMC Short Course on Medicinal Chemistry
Target Selection through Application of Chemical and Systems Biology
April 1-4, 2012
Oegstgeest, The Netherlands
www.efmcshortcourses.org

6th EFMC Short Course on Medicinal Chemistry
Improving Compound Quality: Physical Chemistry and DMPK Properties in Drug Discovery. Principles, Assays and Predictions
October 21-24, 2012
Oegstgeest, The Netherlands
www.efmcshortcourses.org

XXIInd International Symposium on Medicinal Chemistry (EFMC-ISMC 2012)
September 2-6, 2012
Berlin, Germany
www.ismc2012.org

EFMC SPONSORED EVENTS

The 1st Israeli-UK Medicinal Chemistry Conference
April 22-23, 2012, Rehovot, Israel
www.iamc.chemistry.org.il/

30th Noordwijkerhout-Camerino-Cyprus Symposium
May 13-17, 2012
Down-town Amsterdam,
The Netherlands
www.noordwijkerhoutcc2012.com/

15th Hellenic Symposium on Medicinal Chemistry
May 25-27, 2012, Athens, Greece
www.helmedchem2012.gr

21st Italian National Meeting in Medicinal Chemistry
July 17-21, 2012, Palermo, Sicily
www.21nmmc.palermo.it

19th EuroQSAR Knowledge Enabled Ligand Design
August 26-30, 2012, Vienna, Austria
www.euroqsar2012.org

EFMC Sponsored Session at the 4th EuCheMS Chemistry Congress
August 26-30, 2012
Prague, Czech Republic
www.euchems-prague2012.cz/

Annual One-Day Meeting on Medicinal Chemistry of SRC and KVCV
November 2012, Belgium
More information to follow

EFMC SPONSORED SCHOOLS

32nd Edition of the European School of Medicinal Chemistry (ESMEC)
EFMC Accredited School
July 2-6, 2012
Urbino, Italy
www.esmec.eu

Summer School on Pharmaceutical Analyis (SSPA)
June 10-13, 2012
Rimini, Italy
www.scpaweb.org/

10th Swiss Course on Medicinal Chemistry
October 14-19, 2012
Leysin, Switzerland
www.swiss-chem-soc.ch/smc/leysin/leysin.html

Information on the other EFMC sponsored schools which will be organised in 2012 is not available yet, but we invite you to regularly visit the EFMC website www.efmc.info to find out more on the dates and the programmes of the Schools.

Calls for 13 free participations

European School of Medicinal Chemistry (ESMEC), Urbino 2012

The Scientific Committee of the European School of Medicinal Chemistry (ESMEC- Urbino) and the European Federation for Medicinal Chemistry (EFMC) offers 13 (10 + 3) scholarships for the participation to the XXXII edition of the school, scheduled from 2-7 July, 2012.

The scholarships, covering the registration fee and the full board accommodation, will be assigned to PhD students enrolled in Doctoral Schools held in one of the member countries of EFMC, excluding Italy.
A Committee formed by the Director of ESMEC-Urbino, Prof. Gerhard Ecker, representative of EFMC, and Antonello Mai, member of the School's Scientific Committee, will carry out the selection on the basis of the candidate scientific CV.

To apply for a free registration for ESMEC, please fill in the ESMEC grants application form available on www. efmc.info and send it, within April 5th 2012, together with a CV, a motivation letter and an abstract to:
Prof. **Carlo De Micheli**
Dipartimento di Scienze Farmaceutiche
Università di Milano Via Mangiagalli, 25 20133 Milano Italy
mail: carlo.demicheli@unimi.it

XXVIII Edition of the European School of Medicinal Chemistry (ESMEC)
July 2-7,2012 Urbino, Italy
www.esmec.eu

22nd International Symposium on Medicinal Chemistry (ISMC) EFMC–Bentham Travel Grants

The EFMC has reached an agreement with Bentham Science Publishers (www. bentham.org) for the establishment of the EFMC-Bentham Travel Grants with the aim of supporting the participation of young scientists in the ISMC2012. Bentham is funding such travel grants with the sum of 5000 Euros.
The grants will be offered to ten young scientists (500 Euros each), not older than 30 years, who will be nominated by the ISMC2012 Organizing Committee. Applications have to be sent by e-mail to secretariat@ismc2012.org including the CV of the candidate, a supporting letter of a senior scientist and the abstract of the communication. The deadline for submissions is April 2, 2012.

Bentham Science Publishers
www.bentham.org

News from the Societies

BY ERDEN BANOGLU

SPANISH SOCIETY OF MEDICINAL CHEMISTRY

X Seqt Mini-Symposium "Highlights In Drug Discovery From Academia To Industry"

October 25-26, 2012
Segovia, Spain
The Organizing Committee cordially invites you to register for the 10th SEQT Mini-symposium "Highlights in Drug Discovery from Academia to Industry" which will be held in Segovia (Spain) in October 25-26 of 2012 organized by the Spanish Society of Medicinal Chemistry. More information is available on www.seqt.org

HELLENIC SOCIETY OF MEDICINAL CHEMISTRY

15th Hellenic Symposium on Medicinal Chemistry (HSMC-15)

The 15th Hellenic Symposium on Medicinal Chemistry (HSMC-15) will be held on May 25-27, 2012 in Athens at the National Hellenic Research Foundation, The Symposium is organized by the Hellenic Society of Medicinal Chemistry (HSMC) and the Division of Organic and Medicinal Chemistry of the Association of Greek Chemists (DOMC/AGC) and is an EFMC sponsored event.
HSMC-15 continues the tradition of biannual meetings established since more than 25 years in Greece, as a forum for the discussion of recent advances in the field of Medicinal Chemistry.
The topics of the Symposium include drug design and lead identification and optimization, covering all therapeutic areas, as well as the impact of ADME/Tox properties and QSAR in drug discovery. Organic Synthesis, Natural Products, Biochemistry and Chemical Biology, Pharmacology, Computational Chemistry and Chemoinformatics are integrated to create the environment for fruitful interchange of ideas between scientists involved in Medicinal Chemistry as a multidisciplinary research area. Distinguished speakers have been invited to share their views and latest research results, while a round table discussion on the interdisciplinarity in Medicinal Chemistry education is foreseen.
The official language of the Symposium is English. More detailed information and the preliminary scientific program are available in the website at www.helmedchem2012.gr

THE MEDICINAL CHEMISTRY SECTION OF THE ISRAEL CHEMICAL SOCIETY

The 1st Israel-UK Medicinal Chemistry Conference Rehovot, Israel, April 22-23, 2012

The Organising Committee cordially invites you to register for the 1st Israel-UK Chemistry Conference; two days of exciting talks covering a broad range of Medicinal Chemistry including:
– Applications of New Technologies
– Examples of New Approaches in Drug Discovery
– Innovative Clinical Candidates
The scientific programme as well as the registration details are available on the symposium website www.iamc.chemistry.org.il

EFMC | ISMC 2012

XXIInd International Symposium on Medicinal Chemistry

Berlin, Germany September 2-6, 2012

SESSIONS AND SESSION COORDINATORS

ANTIBODY-DRUG CONJUGATES FINALLY READY FOR PRIME TIME? (ACS SESSION I)
Gene Dubowchik (BMS, USA)

ANTI-INFECTIVES AND THE RESISTANCE PROBLEM
Maurizio Botta (University of Siena, IT)

CHALLENGES AND OPPORTUNITIES FOR DRUG METABOLISM IN DRUG DISCOVERY AND PRECLINICAL DRUG DEVELOPMENT (AFMC SESSION)
John Miners (Flinders Unuversity School or Medicine, AUS)

HOT TRENDS IN PROCESS CHEMISTRY
Vittorio Farina (Johnson and Johnson Pharmaceutical R&D, BE)

CHEMICAL BIOLOGY APPROACHES IN DRUG DISCOVERY
Craig Crews (Yale University, USA)

CHEMISTRY AND STEM-CELL RESEARCH SMALL MOLECULE MODULATION OF STEM CELLS FOR REGENERATIVE MEDICINES
Angela Russell (University of Oxford, UK)

DESIGNING BETTER DRUGS: LIGAND EFFICIENCY GUIDED OPTIMIZATION IN DRUG DISCOVERY (ACS SESSION II)
Kap-Sun Yeung (BMS, USA)

EMERGING DRUGS – CASE STUDIES OF RECENTLY DISCLOSED NEW MEDICINES
Rui Moreira (University of Lisbon, PT)

EPIGENETICS – AN AREA OFFERING FORMIDABLE CHALLENGES AND OPPORTUNITIES FOR MEDICINAL CHEMISTS
Dash Dhanak (GlaxoSmithKline, USA)

FIRST TIME DISCLOSURES
Katarzyna Kiec-Kononowicz (Jagiellonian University, PL)

DRUG SAFETY: WHAT TOXIC EFFECTS CAN BE REASONABLY PREDICTED?
Thomas Steger-Hartmann (Bayer Pharma, DE)

INTRACTABLE TARGETS: IS BIGGER BETTER?
Herbert Waldmann
(Max Planck Institute of Molecular Physiology, DE)

LATE BREAKING NEWS
Pascal George (Independent Scientific Expert and Adviser, FR)

METABOLIC DISORDERS
Peter Mohr (F. Hoffmann-La Roche, CH)

MOLECULAR THERAPIES FOR INFLAMMATORY AND AUTOIMMUNE DISEASES
Graham Warrellow (UCB, UK)

NEW DEVELOPMENTS IN CNS DRUG RESEARCH
Anabella Villalobos (Pfizer, USA)

FIGHTING CANCER : KINASES AND BEYOND
Carlos Garcia-Echeverria (Sanofi Aventis, FR)

NEW OPPORTUNITIES IN LEAD DISCOVERY
Gerhard Klebe (Philipps-University Marburg, DE)

NEW SMALL MOLECULE APPROACHES FOR NEGLECTED DISEASES
Jeremy Burrows (Medicines for Malaria Venture, CH)

NEXT GENERATION OF CARDIOVASCULAR DRUGS
Hanno Wild (Bayer Pharma, DE)

STRATEGIES TO TACKLE CHALLENGING TARGETS IN ONCOLOGY
Martin Missbach (Novartis, CH)

PREDICTIVE TOOLS, VIRTUAL SCREENING AND CHEMINFORMATICS
Andy Davis (AstraZeneca, SE)

RECENT HIGHLIGHTS IN MEDICINAL CHEMISTRY
Maria Luz Lopez-Rodriguez
(Complutense University of Madrid, ES)

SYNTHETIC CHEMISTRY: FROM NANO TO MACRO (EUCHEMS SESSION)
Peter Matyus (Semmelweis University, HU)

TARGETING PROTEIN-PROTEIN INTERACTIONS
Kristian Strömgaard (University of Copenhagen, DK)

THE IMPACT OF TRANSPORTERS IN DRUG DISCOVERY AND ORAL BIOAVAILABILITY ENHANCEMENT (EUFEPS SESSION)
Andreas Link (University of Greifswald, DE)

WHAT'S NEW IN GPCR RESEARCH?
Ad Ijzerman
(Leiden/Amsterdam Center for Drug Research, NL)

CONFIRMED PLENARY LECTURES

Ada YONATH
(Weizmann Institute, IL)
Youssef BENNANI
(Vertex Pharmaceuticals, USA)
Günther STOCK
(Health Capital Berlin, DE)
Rainer METTERNICH
(F. Hoffmann-La Roche, CH)

EFMC AWARD LECTURES

– The Nauta Award for Pharmacochemistry
– The UCB-Ehrlich Award for Excellence in Medicinal Chemistry
– The Prous Institute-Overton and Meyer Award for New Technologies in Drug Discovery

EFMC PRIZE LECTURES

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EFMC European Federation for Medicinal Chemistry

DPhG Deutsche Pharmazeutische Gesellschaft e.V.

GDCh Gesellschaft Deutscher Chemiker