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MedChemWatch

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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.
Dear colleagues,

While most of you have received this newsletter through the usual e-mail alert system, someone may have discovered it by flipping through the pages of the first issue of MedChemComm, the official journal of EFMC, launched by the Royal Society of Chemistry, which is now out with the first scientific contributions. Starting with this issue, MedChemWatch will be distributed together with MedChemComm by keeping its traditional quarterly release. The collaboration between MedChemComm and MedChemWatch is meant to provide a stronger link between cutting-edge scientific dissemination and the activities promoted by EFMC and National Organizations.

The Perspective article in this issue of MedChemWatch is expected to be a particularly interesting one. Gerhard Ecker and Koen Augustyns, President and Secretary of the EFMC, comment on the role of medicinal chemistry in the 21st century, and try to take on the challenge of redefining the boundaries of medicinal chemistry in the context of emerging new disciplines like chemical biology and chemogenomics. I am sure that this Perspective will provoke discussion, and I invite all of you to use the newsletter as a tool for exchange of ideas and opinion.

This issue of the newsletter is the last one before the XXI International Symposium of Medicinal Chemistry (ISMC), which will be held in Brussels, September 5-9. The EFMC-ISMC is the biannual world’s largest Medicinal Chemistry meeting and will be articulated in a series of sessions of exceptional scientific level. You may find the final program at www.ismc2010.org, and you are still on time to register.

The ISMC is also the occasion for our community to recognize, though Awards and Prizes, outstanding scientists who have had a significant impact on medicinal chemistry. MedChemWatch has the honor to present the winners of the Awards and Prizes. In this issue, we present the biographical sketch of Camille Wermuth (University Louis Pasteur Strasbourg and Prestwick Chemicals), winner of the Nauta Award, Tony Wood (Pfizer Global Research and Development), recipient of the UCB Award, and Klaus Müller, winner of the Prous Institute-Overton and Meyer Award for New Technologies in Drug Discovery. We are also proud to present the scientific activity and the lab of the two young winners of the newly established EFMC Prizes, namely Andreas Bender, for the academia, and Antonio Nardi for the industry.
The series of the lab presentation is completed by the contribution from iNovacia AB, Stockholm, Sweden.

As usual, the newsletter contains news from the societies, and from the Executive and other Committees of the EFMC. In particular, there are two new functionalities that have been implemented in the official web site of EFMC (www.efmc.info) and that I am sure will be of great utility to our community. The first one is the Meeting Calendar which offers a quick way to organize our schedule for the forthcoming months, and provides us with the chance of not missing an interesting event. The second functionality is the Job Portal, which can be used to publicize open positions, in both academia and industries.

Lastly, check out the news opportunities launched by EFMC to support the participation of young academic scientists to EFMC organized events.

My best regards,

Gabriele Costantino, Editor of MedChemWatch
IUPAC defined in 1998 Medicinal Chemistry as a chemistry-based discipline, also involving aspects of biological, medical and pharmaceutical sciences. It is concerned with the invention, discovery, design, identification and preparation of biologically active compounds, the study of their metabolism, the interpretation of their mode of action at the molecular level and the construction of structure-activity relationships. Is this still a valid definition or should it be modified?

Within the past decade a lot of buzz words, such as chemogenomics, chemical genetics, chemical biology, pharmacoepigenetics, pharmacogenomics, chemical proteomics, systems chemical biology, chembioinformatics, came up which claim to be independent fields or disciplines related to drug discovery and development. With this perspective we would like to provoke a discussion on the future role of medicinal chemistry in the drug discovery and development process as well as give some thoughts on its definition.

**Chemical Biology: An Exciting Challenge For Medicinal Chemists**

The Royal Society of Chemistry defined Chemical biology as both the use of chemistry to advance a molecular understanding of biology and the harnessing of biology to advance chemistry. It is obvious that there is a great deal of overlap between these two scientific fields. Certainly the design, synthesis and characterisation of chemical probes that are used to study and manipulate biological systems, is best performed by experienced medicinal chemists in the classical definition. However, one needs to be aware that good drugs and good chemical probes must meet different criteria. Therefore the focus of a medicinal chemist in classical medicinal chemistry or in chemical biology will be different. Potency is important in both cases, but after that the requirements diverge significantly. Drugs must prove themselves in clinical trials with a desirable clinical outcome. Next to their pharmacodynamic properties, favourable pharmacokinetic parameters and absence of toxicology are required. The degree of selectivity of a drug for a particular protein tar-
Chemogenomics versus "Classical" Drug Discovery

Chemogenomics, in its broadest sense, has been defined as the discovery and description of all possible drugs to all possible targets. This is far beyond any reality, but in a more realistic scenario still should lead to the identification of ligands for all important proteins. With this definition chemogenomics makes a claim that touches the central aim of medicinal chemistry. However, statements like those above by no means account for the complexity of any drug discovery attempt. Generating selective agonists for GPCRs or highly selective inhibitors of ABC-transporters remains quite challenging and is far from being solved. A somewhat different definition of chemogenomics is that it refers to the perturbation of biological systems with the help of small molecules, thus gaining a holistic understanding of the interaction of these molecules with complex biological systems. This emphasises the more technological part of chemogenomics with its automation and miniaturisation attempts and is more in line with all the other "-omics" approaches. According to this definition, chemogenomics is thought to help to identifying the respective molecular targets of these compounds. Therefore, rather than following the long lasting paradigm of starting with the target to find the drug, chemogenomics should generate drugable targets.

Implementation of these technologies certainly will aid in our understanding how drugs work. With the few of a medicinal chemist, chemogenomics provides new tools and techniques which will support the medicinal chemist scaling his or her lead generation and optimisation capabilities from single experiences towards a more broader and systematic understanding of the interaction of small molecules with biological systems. Being per se molecular driven, also chemogenomics has a lot of overlap with medicinal chemistry and thus offers great opportunities for our involvement.

These are two examples of new fields of research, which have been established and which have considerable overlap with medicinal chemistry and in some cases even have been started out of "classical" medicinal chemistry. These new research fields have a merit of their own, but also contribute to the continuous development of what medicinal chemistry is, and what future drugs should look like. While classical drug discovery and development and understanding structure activity relationships are still the core of medicinal chemistry, the field has developed a lot,
including much more than the classical definition indicates.

**Medicinal Chemistry and the Innovative Medicines Initiative**

In 2008, the governing board of IMI – The Innovative Medicines Initiative – approved the strategic research agenda of this World’s largest public private partnership with a volume of 2 billion € for the next 7 years. The IMI Research Agenda is a multiannual plan developed by the European Technology Platform on Innovative Medicines which identified principal research bottlenecks in the biopharmaceutical R&D process and sets forth recommendations to overcome these bottlenecks by focusing on four areas: predicting safety, predicting efficacy, knowledge management, and education and training. Main disease areas targeted are cancer, brain disorders, metabolic disease, inflammation and infectious diseases.

The research projects proposed by IMI are broad and multi-disciplinary and thus cannot be carried out by one company or within one member state. One main characteristic of IMI is that projects are also ‘precompetitive’ for the pharmaceutical industry. Companies (including SMEs), academics, regulators and patients need to come together to share resources and expertise to address the challenges of drug discovery and development (www.imi-europe.org). Results and the knowledge and capabilities gained from performing such projects should be made available to the entire public and private sector. For example, the call for an open pharmacological space (knowledge management call round 2) should lead to an open data open access system where you can answer questions like “give me all compounds inducing cholestasis and their profiles at liver transporters” just with typing in one query! This will revolutionise the way how data can be mined in medicinal chemistry projects.

There was a lot of discussion within EFMC that IMI is not made for medicinal chemists, as medicinal chemistry is considered a core discipline in drug discovery, thus being purely competitive. However, as outlined above, medicinal chemistry knowledge is required in a lot of areas considered to be precompetitive, such as chemical biology and chemogenomics. Thus, there are many opportunities for medicinal chemists and the projects approved in the first call showed already that there is plenty of space for medicinal chemistry groups.

**Outlook**

The science of medicinal chemistry has been used since more than 100 years for the discovery and development of new safe medicines. The field has become increasingly dynamic and medicinal chemists face the challenge of rapidly evolving new technologies. One of the next large steps will be the “virtualisation” of the field. The Swiss branch office of PricewaterhouseCoopers recently published an analysis that greater use of new technologies to virtualise the research process and accelerate clinical development will reduce the number of clinical studies by 40% and the number of patients in clinical studies by 65%. Whether real or virtual, finally it comes down to chemical entities and their interactions, which are driven by the basic laws of physicochemistry. EFMC is ready to take the challenge of being the central hub for these developments. With its symposia, short courses and schools, its newsletter and now also with MedChemComm, EFMC provides perfect conditions for exchanging and promoting new ideas, exploring new grounds and moving beyond established thinking!
iNovacia AB, Stockholm, Sweden, was created in 2006 as a scientist buy-out from Biovitrum, which in turn was a spin-out in 2001 from Pharmacia Corporation. iNovacia is now an established drug innovator providing discovery services to pharmaceutical and biotech companies in Europe and the US. We specialize in providing competitive preclinical candidates applying technologies to build a strong foundation for the understanding of structure-activity relationship and predictive ADMET.

iNovacia offers a complete coverage of early drug discovery steps from assay development to optimized leads and IND state. Services include assay development, high-throughput screening (HTS), fragment-based screening by NMR and SPR, analytical chemistry, medicinal chemistry at all stages up to lead optimization, ADMET profiling and biophysical characterization of proteins and compound-protein interactions.

iNovacia scientists are using a range of biophysical techniques to decipher and validate mechanism of actions of hit series from HTS. The picture shows the high field NMR-laboratory.

The highly experienced HTS team has performed screening campaigns towards all major target classes (GPCRs, ion channels, enzymes, nuclear receptors) using a wide range of assay read-outs (e.g. radioactivity, fluorescence, luminescence, absorbance). Primary fragment screening is performed by ligand-based NMR techniques or SPR using a 900+ fragment library.

The hit-to-lead phase where the most promising hit series are selected for further development in full medicinal chemistry programs is a crucial step for a successful drug discovery project. iNovacia devotes much efforts to ensure that the medicinal chemists work on the most promising hit series. Counter assays and orthogonal assays are employed and our medicinal chemists evaluate the hit series with respect to chemical tractability, library expansion tractability, emerging SAR and IP space. Whenever possible, biophysical assays are performed on hit series representatives in order filter out series active via an undesired mechanism and also to obtain more information on binding modes of compounds from promising hit series. Further, analogues are tested and selected series are expanded by parallel chemistry. Finally, early in-vitro ADME assays are performed before the final prioritization of hit series and continuation of the project into the lead-generation and lead-optimization phases.

iNovacia has several modular service offerings that can be used separately or combined. A combination of the modular offerings can for example cover all steps from assay development to the hit-to-lead phase. iNovacia brings an integrated drug discovery organization underpinned by an investment of 10 Mio EUR in instruments and over 15 years of industrial track record of delivering drugs into the clinic and onto the market.
MedChemWatch has the honor to acknowledge the winners of the EFMC Awards. In this issue, we present a short biographical sketch of Camille Wermuth, Université Louis Pasteur Strasbourg and Prestwick Chemicals, winner of the Nauta Award for Pharmacochemistry, Tony Wood, Pfizer Global Research and Development, Sandwich UK, winner of the UCB-Ehrlich Award for Excellence in Medicinal Chemistry and Klaus Müller, Roche-ETH Zurich, winner of the Prous Institute-Overton and meyer Award for New Technologies in Drug Discovery.

NAUTA AWARD
FOR PHARMACOCHEMISTRY

Camille G. Wermuth

Camille G. Wermuth was for more than three decades Professor of Organic and Medicinal Chemistry at the Faculty of Pharmacy at the Louis Pasteur University in Strasbourg, France.

He became interested in Medicinal Chemistry during his two years of military service in the French Navy at the “Centre d’Études Appliquées à la Marine” in Toulon. During this time, he worked under the supervision of Dr. H. Laborit, the scientist who invented artificial hibernation and discovered chlorpromazine. Later he created and headed for 27 years the Molecular Pharmacochemistry Unit of the CNRS (“Centre National de la Recherche Scientifique”) in Strasbourg. This unit was original in that it had three areas of responsibility: synthetic organic chemistry, medicinal chemistry and computer modeling.

His research has led to the development and synthesis of many research tools for the Neurosciences and to the development of a new psychotropic drug, minaprine, marketed in Europe since 1980. His interests focussed on GABAergic and cholinergic drugs, dopamine D₃ receptor ligands, and CRF receptor antagonists.

Professor Wermuth is the author and co-author of over 300 peer-reviewed scientific papers. He holds over 60 patents. He is the author, co-author, and editor of several books or book chapters. His most recent book, “The Practice of Medicinal Chemistry,” first published in 1996, and now published in the third edition, was translated into several languages, including Japanese and Chinese.

Besides his academic career he was always interested in industrial collaborations and drug discovery projects. This resulted in the foundation of the medicinal chemistry company Prestwick Chemicals in 1999 in which he put all his efforts after retirement from University. He became President and Chief Scientific Officer of the company and was responsible for the success of the company. Over the years Prestwick was continuously growing and has now more than 30 employees.

Professor Wermuth has been awarded the Charles Mentzer Prize of the Société Française de Chimie Thérapeutique, the Léon Velluz Prize of the French Academy of Science, and the Prix de l’Ordre des Pharmaciens by the French Academy of Pharmacy. He is Corresponding Member of the German Pharmaceutical Society, and was nominated Commandeurs des Palmes Académiques.

He has been nominated President of the Division of Chemistry and Human Health of the International Union of Pure and Applied Chemistry (IUPAC).

On the occasion of the 21th International Symposium on Medicinal Chemistry 2010 in Brussels he will be awarded with the Nauta Award.
Tony Wood is Vice President and Head of Worldwide Pfizer Medicinal Chemistry, Pfizer.

Tony Wood has been named as the 2010 winner of the prestigious UCB-Ehrlich Award for Excellence in Medicinal Chemistry. The award is conferred by the European Federation of Medicinal Chemistry (EFMC) every two years to acknowledge and recognize outstanding research in the field of medicinal chemistry in its broadest sense by a young scientist.

Tony Wood was selected as the 2010 recipient by an International Selection Committee, in part, due to his leading the discovery of maraviroc, Pfizer’s breakthrough therapy for HIV infection and the first small molecule antagonist of the CCR5 receptor. In addition to his role guiding Pfizer’s strategy for medicinal chemistry, Tony Wood is an active member of the scientific community and demonstrates a commitment to medicinal chemistry education through a number of external roles.

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Tony Wood received his BSc in 1987 and PhD in 1990 in chemistry from Newcastle University, before completing post-doctoral studies with Professor Steven Ley, FRS at Imperial College in London working on the total synthesis of azadirachtin, one of the most complex molecules ever to have been synthesised, and a project that has only recently been completed.

Tony Wood has active interests in many areas of medicinal chemistry including G-protein coupled receptors, cyclic nucleotide processing enzymes, nucleoside and non-nucleoside antiviral drugs, serine and aspartyl protease inhibitors, protein transferases and kinases, protein-protein interactions and transcription factor regulation. Tony Wood is particularly interested in HIV, HCV and HPV therapies, and molecular virology from the standpoint of intervention of modulation of host targets, in particular the cellular targets necessary for viral fusion and activation of viral transcription.

Tony Wood has a highly successful track record of compound design and candidate delivery, including broad-spectrum antifungal agents, sub-type selective GPCR antagonists and potent cyclic nucleotide phosphodiesterase enzyme inhibitors. He has also been involved in the application of high-throughput synthesis and screening technologies to improve efficiency in drug discovery, and the use of yeast genomics to identify new targets for therapeutic intervention.

Tony Wood has held positions on a number of UK funding council review boards such as the BBSRC and EPSRC, and has recently been elected to the EPSRC’s Council, its top-level strategic committee. Tony Wood is co-editor in chief of the new RSC journal, Medicinal Chemistry Communications, and was editor of volume 41 of Annual Reports in Medicinal Chemistry in 2006. Tony Wood is an author or inventor on more than 50 scientific publications and patents, and has given invited lectures at a number of International Conferences on Medicinal Chemistry. Tony Wood is also a Visiting Professor at Newcastle University.

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Klaus Müller studied chemistry at the ETH Zurich, where he obtained his Ph. D. degree in 1970 with Prof. Albert Eschenmoser. After postdoctoral work with Prof. Gerhard L. Closs at the University of Chicago, studying radical reactions by nuclear magnetic resonance spectroscopy (CIDNP), he moved to Harvard University as a visiting lecturer (1971-1974) on physical and theoretical organic chemistry.

By the end of 1974, he joined the scientific staff of the Laboratorium für Organische Chemie at ETH Zurich, where he did his Habilitation in 1977, focusing on molecular structure, energy, reactivity relationships and investigating the chemistry of a series of novel strained heterocycles, using photoelectron spectroscopy.

In 1982, he joined F. Hoffmann-La Roche AG, Basel, in order to set up a molecular modeling group and to help implement biostuctural research using macromolecular X-ray and multi-dimensional NMR spectroscopic analyses. In 1988, he became head of the Section “Computer-Assisted and Structural Chemistry, and, in 1991 head of the Department of “Pharma Research Logistics & Support” and “Pharma Discovery Information Management”.

In these various functions, he has been instrumental in implementing and further developing computer-assisted molecular modeling and, together with Dr. Paul Gerber, developed the MAB force field and the molecular modeling software “MOLOC” that is today widely used not only at Roche but also in academics and other pharmaceutical companies.

During that period, Klaus Müller pushed computational chemistry, bioinformatics, structure-property analytics and correlation methodologies, bringing some of the finest scientists aboard at Roche and fostering intimate contacts with academia.

Since early 1998, he has been head of “Science & Technology Relations” in Pharmaceutical Research at Roche, Basel. In this function, he has acted as liaison person to both academic institutions and non-academic external groups and has been responsible for the search and early identification of young talents in chemistry and the life sciences. He founded the annual “Roche Symposium for Leading Chemists of the Next Decade” which rapidly became a honoring entry into the CV of those who were selected from all of Europe to attend.

He was a board member and Secretary-General of the Roche Research Foundation from 1999 till its conclusion at the end of 2008. Since 1990, he is Extraordinary Professor at the University of Basel, giving advanced courses on “Structure- and Property-Guided Molecular Design”; a lecture series that he also presented at ETH and, as invited “Robert B. Woodward Visiting Scholar”, in 2006 in the Department of Chemistry and Chemical Biology at Harvard University. He was promoted in Spring 2005 to “Roche Distinguished Scientist”, one of the first in this novel and highest scientific promotion category of Roche. After his regular retirement in Spring 2009, Klaus Müller continues to be affiliated with Roche as a consultant in chemistry and scientific matter, managing among others the new Roche Postdoctoral Program. At the same time, he has resumed his teaching activities at the ETH Zurich where he gives the main upper level “Physical Organic Chemistry” course.

Most importantly, over all these years, Klaus Müller has always been able to pursue his own research projects targeting the generation and introduction of new concepts in structure-based lead discovery and optimization. These scientific achievements are documented in more than 80 publications and in over 250 lectures, mostly scientific but also on science policy matters.
Antonio Nardi

Winner of the EFMC Prize for Young Researcher in Industry

Dr. Antonio Nardi (1976, married, two children) graduated at the faculty of Pharmacy of Pisa University in 2001 (Italy), awarded the same year with the Virdis prize as outstanding graduate and obtained in 2005 a PhD in medicinal chemistry from the same university. Throughout the course of his doctoral studies (2001-2004), first under the supervision of Prof. Biagi Giuliana at the Department of Pharmaceutical Sciences in Pisa (www.farm.unipi.it/scieweb) and later under the supervision of Dr. Rodriguez Sarmiento Rosa Maria at the Pharmaceutical Division, Discovery Chemistry at Hoffmann-La Roche AG in Basel (Switzerland) (www.roche.com), Dr. Nardi had the opportunity to come into contact with diverse drug targets and a number of therapeutic areas.

His main research interest, though, focused on the design and synthesis of structurally novel heterocyclic compounds as modulators of potassium channels, especially the large-conductance calcium-activated potassium channels (BK), and their potential therapeutic application in cardiovascular diseases.

His research efforts in this field were then further advanced at NeuroSearch A/S (www.neurosearch.com) (Ballerup, Denmark), a biopharmaceutical company focused on unmet medical needs and a well-known and recognised pioneer in the BK channel field. Dr. Nardi first served there as a post doc and subsequently as a research chemist leader for the BK channel programme (2005-2010).

His work has resulted in the design of modulators that are currently among the most potent BK channel openers (whose status cannot be fully disclosed) as well as in the identification of new tool compounds (such as NS11021 and NS13558) that are currently the basis for scientific collaborations with several American and European universities and research centres and by which the therapeutic potential of BK channels in conditions as diverse as ischemia, chronic obstructive pulmonary disease (COPD), erectile dysfunction and overactive bladder is currently investigated. One of such research centre is the Danish Arrhythmia Research Centre (DARC), in Copenhagen (Denmark) (www.darc.ku.dk), where he is currently appointed visiting professor in medicinal chemistry.

At NeuroSearch, besides the research in the field of BK channel modulators, Dr. Nardi has also extended his scientific interests to positive allosteric modulators of nicotinic acetylcholine receptors, for which research programme he served as a research chemist leader throughout hit selection and advanced lead optimisation phase, as well as he had the opportunity to launch a new research programme in drug discovery, for which he served both as a chemistry leader and project leader. This program is to be considered distinctive in that it is carried out very much in opposition to the most classical paradigms of the modern drug discovery. Part of this uniqueness is due to the fact that only high-quality compounds, designed upon a semi-rational principle, are tested in a primary in vivo screening and their potential in a given therapeutic indication, irrespective of the molecular target(s), is explored by means of systems biology approaches.

As per March 1st 2010, Dr. Nardi (antonio.nardi@grunenthal.com) has taken up a position within the Preclinical R&D division (Medicinal Chemistry) at Grünenthal (www.grunenthal.com) in Aachen (Germany) where he is currently Associate Scientific Director and serves as Project Manager of a research programme aiming at a novel type of ion channel modulators.

Dr. Nardi has authored more than 15 peer-reviewed articles and is (co)inventor in more than 20 patent applications.
10 Years in the Cheminformatics Field – From a Start-Up in Berlin to a Lectureship in Cambridge

There are times in life where you make consciously the right decision - but there are also those situations where a seemingly random choice turns out to be the exactly right one in hindsight. In my case, after studying chemistry at Technical University Berlin and returning from an exchange year at Trinity College Dublin, I had the summer after my year abroad off – and having been the decent student I was I decided to look for an internship in a related field. Now, originally I planned to work in South America in summer, but realizing the preparations required for this step I settled for an internship with a cheminformatics start-up close to Berlin instead, in Hennigsdorf, called CallistoGen.

It was the golden time of biotech, back then in summer 2000 (hard to imagine today probably!), and this was the first time that I was in touch with ligand-based approaches to drug design, giving me a scientific direction for about 10 years by now. While admittedly being neither a computer expert nor capturing every detail of the virtual screening algorithms I helped to develop at that time, this stint made me realize my desire to move away from the bench, and to simulations-based work from now on. (An accident in my chemistry lab at home where I nearly lost my eyesight and which kept me in hospital for over a month might have been a contributing factor as well.)

The nice thing about science is that you can move around relatively freely. Hence, for my Master’s Thesis I went to Goethe University Frankfurt to work with Gisbert Schneider on a bioinformatics topic; while for my PhD I moved to the UK to extend previous work on virtual screening algorithms at the Unilever Centre for Molecular Informatics in Cambridge / UK with Bobby Glen (which, in fact, is also the place I returned to just a few months back to assume a position as a research group leader). What I am very grateful for is a so-called ‘Presidential’ Postdoctoral Fellowship with Novartis in Cambridge / MA afterwards – it is a fantastic program, which allows the postdoc to do essentially three years of independent research, with all the resources a pharmaceutical company can offer. (‘Presidential’ here refers to the head of the research arm of Novartis, not ‘W’ in case you might wonder.)

Given the independent research possible in this position, and under the direction of Jeremy Jenkins, we published more than a dozen papers during my tenure with Novartis, which allowed me to become an Assistant Professor with the Leiden / Amsterdam Centre for Drug Research (LACDR) before assuming my current position as a lecturer with Cambridge University.

Chemogenomics Databases – Millions of Bioactivity Data-points are at our Disposal for Ligand Design Efforts

So why should ligand-based drug design methods be of interest in current days, with more and more crystal structure popping up in databases every day? Well – not only that both methods are often complementary, but there is simply such a lot of ligand bioactivity (and more generally, property) data out there which we can (and should) put to good use for future medicinal chemistry activities. To mention a few numbers: The ChEMBL database at the European Bioinformatics Institute (EBI) which was recently released publicly as one of the biggest databases of this type, contains more than 560,000 compound records with more than 2,700,000 experimental activities in its current release, spanning more than 7,300 targets. (‘Targets’ in this context might be proteins, but also phenotypic readouts such as ‘as ‘walking behaviour’ or ‘change in foot-licking latency’ which are surely some of the more interesting assays to perform). Also other properties, such as lipophilicity or solubility are of interest to the modelling community of course, but I have to say that, personally, I am most interested in the factors that contribute to the activity of chemical matter against protein targets.

This type of data can now be used in multiple ways which are also pursued in my current research group in Cambridge, as well as previously in Leiden, termed ‘chemogenomics’ or ‘proteochemometrics’ approaches. These modelling methods take information about the ligand structure, as well as the target protein, into account in order to make bioactivity predictions. So why is this useful? Well, imagine you have a series of compounds, A1, A2, and A3, which you measure against target 1. At the same time, you know the activities of compounds B1, B2 and B3 against target 2 (see Figure 1 for an illustration). In classical models, you would need to generate two separate
bioactivity models, one for target 1 and one for target 2, each of which covers only a relatively small area of chemical space each. However, if you knew how to translate bioactivities from target 1 into bioactivities against target 2, you would on the one hand cover more chemical space in your model (namely chemical space represented by all of the ligands above), and on the other hand you would learn to be able to extrapolate between targets 1 and 2. You are now thinking of ligand selectivity (or desired promiscuity) profiles against GPCRs? Or bioactivities against highly resistant mutants of viral enzymes? Then you move into the absolutely right direction - these are the typical areas where proteochemometrics research could be applied, and where we will release prospectively validated primary research results in the very near future.

As illustrated in this example, by employing chemogenomics principles – namely relating proteins by the similarities of their ligands - we can use ligand bioactivity data in a much wider way then before. This type of modelling, taking into account up to millions of data points, has applications that range from receptor deorphanization, to the prediction of polypharmacology of compounds against G-Protein Coupled Receptors, to the selection of the right HIV Reverse Transcriptase Inhibitor active against a particular mutant of this enzyme.

From Chemical Space, via Protein Targets and Pathways, to Phenotypes (and back again)

One can even go a step further than this, and not only map chemical space onto biological space: The next logical step, and this is also the plan for future research in my group at Cambridge University, is to include information also about phenotypic space in this concept. This would likely involve two steps, firstly pathways information mapped onto the targets, and secondly including also phenotypic information that is known to be related to modulation of those pathways. A database of this type, schematically displayed in Figure 2, could be used in a myriad ways in drug discovery: Be it in the analytical way, by deconvoluting the mechanistic reasons behind adverse drug reactions, or in the way more relevant for drug discovery, by rationally choosing ligand chemical features in order to modulate targets and pathways in a manner to reverse the diseased phenotype. Being realistic, our knowledge of bioactive chemical space and pathway annotations is overall still very limited – still, we have millions of chemogenomics data points at our disposal, which we can already use today to make more informed decisions on how to modify compounds to achieve the desired, phenotypic effect.

PhD Students and Postdoctoral Positions Open at the Unilever Centre

The above are only examples of the amount of knowledge and the versatility current bioactivity and pathway databases offer to researchers in the life sciences and I would be very happy to contribute with my experience in chemical data mining and retrieval to experimental ligand design projects in research groups anywhere in the world. Given our recent renewal of funding at the Unilever Centre for Molecular Informatics at the University of Cambridge we are currently heavily recruiting about 10 PhD students and postdoctoral fellows in and around the cheminformatics, chemogenomics and metabolism areas. If you are interested you are cordially invited to visit the Unilever Centre website at http://www-ucc.ch.cam.ac.uk/ or my personal departmental website at http://www.ch.cam.ac.uk/staff/ab.html for further information. Also of course, feel free to contact me directly by e-mail at Andreas.Bender@cantab.net if you would like to discuss options for joint research projects or if you are interested in joining our research groups.

**Figure 1.** While for conventional bioactivity models one model per activity class needs to be generated, in proteochemometric models only a single model, covering all related protein targets at once, is required. Advantages are larger coverage of chemical space on the ligand side, plus the ability to extrapolate to novel, but related targets (the extent of which depends on the precise data given).

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<tr>
<th>MULTIPLE CONVENTIONAL BIOACTIVITY MODELS</th>
<th>ONE PROTEOCHEMOMETRIC MODEL</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>COMPOUND</strong></td>
<td><strong>TARGET OTHER</strong></td>
</tr>
<tr>
<td>A1</td>
<td>A2</td>
</tr>
<tr>
<td>COMPOUND</td>
<td>COMPOUND</td>
</tr>
<tr>
<td>B1</td>
<td>B2</td>
</tr>
</tbody>
</table>

**Figure 2.** By integrating chemical space with target and pathway annotations, plus a phenotype definition that depends on the particular study, the wealth of data available today can be used in both directions: to rationalize phenotypic observations of compounds (such as adverse reactions), as well as to influence phenotypes – the objective of every drug discovery programme.
NEWS ON ACTIVITIES FOR 2010

• August 20, 2010
2nd International Symposium on “DNA-Encoded Chemical Libraries” ETH Zürich
Organized by Prof. Dr. Dario Neri

• September 16, 2010
Division of Medicinal Chemistry, oral and poster session at the Fall Meeting of the Swiss Chemical Society ETH Zürich

• September 21-24, 2010
The Swiss Chemical Society will organize the ILMAC Scientific Forum at the Fair Basel (MCH) entitled “From Nylon to Nanomaterials. Future Trends in Polymers”, with a specific section on September 23 dedicated to Biopolymers and Polymer Based Drug Delivery. The program will include a lecture by Prof. Alberto A. Gabizon (Hebrew University, Jerusalem, Israel): “Delivery of Anticancer Agents by Liposomes: Nanomedicine in Action”.

• October 10-15, 2010
9th Swiss Course on Medicinal Chemistry, organized by Professor Beat Ernst in Leysin, a picturesque Swiss mountain village. This course is held every second year. It offers young scientists with a few years of experience in the pharmaceutical industry and interested Ph.D. students a broad overview of key disciplines important for modern pre-clinical drug research. Active participation in tutorials and a broad variety of lectures and case histories are important elements of the course (see also http://www.swiss-chem-soc.ch/events/index.cfm).

NEWS ON ACTIVITIES FOR 2011

• March 20-23, 2011
Joint German-Swiss Meeting on Medicinal Chemistry “Frontiers in Medicinal Chemistry”, Saarbrücken, Germany.

Participation in various events which will be organized to celebrate the UN International Year of Chemistry 2011.

HELLENIC SOCIETY OF MEDICINAL CHEMISTRY

A report on the 14th Hellenic Symposium on Medicinal Chemistry in Thessaloniki, Greece

The 14th Hellenic Symposium on Medicinal Chemistry (HSMC-14) took place in Thessaloniki on 23-25 April, 2010 and was a successful event. It was co-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). This series of Symposia follows the tradition of bi-annual conferences, established since more than 25 years in Greece, as a forum for the discussion of recent advances in the field of Medicinal Chemistry. For the first time HSMC-14 was an EFMC sponsored meeting with pronounced international participation, represented by invited speakers as well as oral presentations and posters from different European countries, among them, the president of EFMC Prof. Gerhard Ecker and the Council member Prof. Danijel Kikelj who also participated in the round table discussion on: Education and Research in Medicinal Chemistry: The role of Universities and the views of industry. In total there were about 150 participants who presented 5 plenary lectures; 11 main lectures 22 oral presentations and 100 posters. The Symposium attracted increased interest from a considerable number of Pharmacy and Chemistry students. A pre symposium workshop on molecular modeling (1st Hellenic Workshop on Molecular Modeling and Molecular Docking) was successfully organized for the first time.

The Symposium focused on different aspects of Medicinal Chemistry balancing from rational design, synthesis and biological evaluation of new compounds, molecular modeling and docking and drug transporters to screening and semi- or total synthesis of natural products as well as to radiopharmaceuticals. The program of the Symposium is still available on the website at www.helmedchem2010.gr

The next scientific appointment for medicinal chemists in Greece will take place in 2012 in Patras and the two organizations, the Hellenic Society of Medicinal Chemistry and the Division of Organic and Medicinal Chemistry of the AGC are already joining their efforts in setting up the 15th HSMC-2012.
SESSIONS AND SESSION COORDINATORS

CAREERS IN MEDICINAL CHEMISTRY
Graeme Robertson (Sienabiothech, Italy)

CHEMICAL APPROACHES TO STEM CELL BIOLOGY
Sheng Ding (The Scripps Research Institute, United States)

CHEMICAL STRATEGIES FOR FUNCTIONAL PROTEOMICS - ACTIVITY-BASED PROTEIN PROFILING
Stephan A. Sieber (Ludwig-Maximilians-Universität München, Germany)

COVALENT INHIBITORS IN DRUG DISCOVERY
Stan Van Boeckel (Schering-Plough, The Netherlands)

EMERGING DRUGS - CASE STUDIES OF RECENTLY DISCLOSED NEW MEDICINES
Nicholas Carruthers (Johnson & Johnson R&D, United States)

EMERGING TECHNOLOGIES
David Parry (Cyclofluidic, United Kingdom)

FINDING THE RIGHT BINDING POCKETS: ALLOSTERIC MODULATORS OF G-PROTEIN COUPLED RECEPTORS FOR NON-CNS DISEASES (ACS Session)
Robert A. Fecik (University Of Minnesota, United States)

FIRST TIME DISCLOSURES
Eckhard Ottow (Bayer Schering Pharma, Germany)

G-PROTEIN COUPLED 7TM RECEPTORS - NEW INSIGHTS INTO THEIR STRUCTURE AND LIGAND RECOGNITION
Hans Bräuner-Osborne (The Danish University of Pharmaceutical Sciences, Denmark)

HOT TOPICS IN ANTI-INFECTIVES
Lieveen Meerpoel (Johnson & Johnson PRD, Belgium)

HOT TOPICS IN CARDIOVASCULAR DISEASES
Joachim Mittendorf (Bayer Schering Pharma, Germany)

HOT TOPICS IN CNS DISEASES
Benoît Kenda (UCB, Belgium)

IMAGING BIOMARKERS
Gilles Tamagnan (Iale School of Medicine, United States)

INNOVATIVE DRUG DELIVERY SYSTEMS AND NANOTECHNOLOGIES (EUFPS Session)
Daan Crommelin (T1 Pharma, The Netherlands)

KNOWLEDGE ENABLED DRUG DESIGN
Mark Bunnage (Pfizer, United Kingdom)

RECENT CASE STUDIES IN DD AND DEVELOPMENT
Gerhard Ecker (University of Vienna and EFMC, Vienna)

MOLECULAR THERAPIES FOR INFLAMMATORY AND AUTOIMMUNE DISEASES: ONGOING CLINICAL TRIALS AND FUTURE PROSPECTS
Sylviane Muller (CNRS Strasbourg, France)

NATURAL PRODUCTS IN DRUG DISCOVERY BEYOND CYTOTOXICS AND ANTI-INFECTIVES
Gloria Serra (Udelar, Uruguay)

NEW MEDICINES BEYOND SMALL MOLECULES
Hans-Ulrich Stilz (Sanofi-Aventis, Germany)

NOVEL TREATMENTS FOR OBESITY AND METABOLIC DISORDERS
Roberto Pellicciari (University of Perugia, Italy)

ONCOLOGY CASE STUDIES
Peter Ettmayer (Boehringer Ingelheim, Austria)

PROCESS R&D AND SCALE-UP: CHEMISTRY, CRYSTALS & MORE CHALLENGES AND SUCCESS STORIES
Herbert Stark (Sanofi-Aventis, Germany)

SUCCESSFUL STRATEGIES IN LEAD DISCOVERY
Hans Peter Maerki (F. Hoffmann – La Roche, Switzerland)

TARGETING PATHWAYS
Nicholas Cosford (Burnham Institute for Medical Research, United States)

TARGETING PROTEIN-PROTEIN INTERACTIONS (AFMC Session)
David Winkler (CSIRO Molecular Science, Australia)

TEACHING MEDICINAL CHEMISTRY
EFMC: Teaching & Training Committee

THE CHALLENGES IN DESIGNING MULTIPLE LIGANDS DRUGS. THE GOOD, THE BAD AND THE UGLY (ACS Session)
John Butera (Wyeth Research, United States)

TOXICITY CHALLENGES IN DRUG DESIGN AND STRUCTURE-TOXICITY RELATIONSHIPS
Ferran Sanz (Universitat Pompeu Fabra, Spain)

VIRTUAL SCREENING AND PROFILING
Didier Rognan (University of Strasbourg, France)
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-ISM C, EFMC-ASMC, Frontiers in Medicinal Chemistry, EFMC Short Courses or the EFMC Accredited School will be covered by EFMC. Applications should reach the Administrative Secretariat (administration@efmc.info) at least six weeks prior to the event and should consist of a CV and a short motivation letter. 

The EFMC website offers links to the job portals of EFMC corporate members as well as information on current vacant positions. The posting of job offers is free and is available for any medchem related jobs, in industry as well as academic positions. To have your job offer published on the website, please fill in the application form available on the site (http://www.efmc.info/content.php?langue=english&cle_menus=1199870681).

We also invite you to have a look at the renewed meeting calendar, aimed to become a one stop shop for all medicinal chemists. Monthly tabs and a search function give you the possibility to navigate easily through the list of worldwide organized medchem events. The calendar is updated and completed on a regularly basis (http://www.efmc.info/summary-events.php?langue=english&cle_menus=1113380777).

At the Council Meeting, which will take place on occasion of the XXI International Symposium on Medicinal Chemistry (September 5-9, 2010), the council will elect 6 positions for the Executive Committee. The positions to be elected are president-elect, treasurer, secretary, and three additional members. The terms for all the elected EC-members will start on Jan 1st, 2011 and last for two years. The president-elect will automatically become President on Jan 1st, 2012.

The EFMC Council will also decide on the organizers of the 2014 edition of the International Symposium on Medicinal Chemistry. EFMC is the initiator and sponsor of this series of symposia, each of which is organized in a European city in collaboration with one or more EFMC National Adhering Organization(s).

ISMC 2012 will be held in Berlin.

EFMC Short Course
After the success of the first EFMC Short Course in 2009 at Kasteel Oud Poelgeest near Leiden in the Netherlands, it was decided to organise further short courses at regular intervals in the same centre. Aimed primarily at Medicinal Chemists in industry it was also decided these would all be at an advanced level. The second short course in the series covering Safety and Attrition was held from 11-14 April 2010. Alan Stobie (Pfizer UK) was responsible for the programme and selection of the contributors. Alan and Henk Timmerman acted as course directors. The course, like the first one, was fully booked with 34 participants, most of whom were from European, but with some from as far away, as Canada and Singapore. Most participants were from industry, but there were also two academics. The course was a major success, with participants enthusiastic about the programme, the quality of the lectures and the venue. Most of the lecturers stayed for the whole of the course, allowing intensive discussions with the participants. The course was “evaluated” by means of a questionnaire; with individual contributions scored by participants for both contents and for quality of the presentation on a scale 1 (poor) to 5 (excellent). The score of all contributors was very high with an average of 4.35 for quality of the presentation and 4.18 for the contents.

A third short course will be announced later this year and will most likely occur in April 2011.
EFMC-ISMC 2010
21ST INTERNATIONAL SYMPOSIUM ON MEDICINAL CHEMISTRY

Date: September 5-9, 2010
Place: Brussels, Belgium

Website: http://www.ismc2010.org

EFMC-ISMC 2010 will be organised by the Medicinal and Bioorganic Chemistry Division of Royal Flemish Chemical Society (KVCV) and the Division for Medicinal Chemistry of the Société Royale de Chimie (SRC), on behalf of the European Federation for Medicinal Chemistry (EFMC). This symposium traditionally attracts experts in drug research and development, in particular medicinal and synthetic chemists, combinatorial chemists, molecular modelers, pharmacologists, as well as development chemists. It is is recognized worldwide as one of the leading Medicinal Chemistry meetings, as proven by its large international attendance.

Contact:
Dr. Edmond Differding
Email: edmond.differding@belgacom.net

Organised by:
The European Federation for Medicinal Chemistry (EFMC) and by the Medicinal and Bioorganic Chemistry Division of Royal Flemish Chemical Society (KVCV) (Belgium) and the Société Royale de Chimie (SRC), Medicinal Chemistry Division (Belgium)

XXST NATIONAL MEETING ON MEDICINAL CHEMISTRY
OF THE DIVISION OF ITALIAN CHEMICAL SOCIETY

Date: September 12-16, 2010
Place: Padova, Italy

Website: http://www.nmmc2010.sistemacongressi.com/

Topics:
CNS Medicinal Chemistry
Epigenetics: A New Pathway to Drug Discovery
Oncology Medicinal Chemistry
Antibacterial and Antiviral Agents
Pharmaceutical Profiling Assays in Drug Discovery and Development
Drug Design

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Organised by:
Division of Medicinal Chemistry of the Italian Chemical Society (Società Chimica Italiana) (Italy)
18TH EUROPEAN SYMPOSIUM ON QUANTITATIVE STRUCTURE – ACTIVITY RELATIONSHIPS

Date: 19-24 September 2010
Place: Rhodes, Greece

Website:
http://www.euroqsar2010.gr

Topics:
Pharmacophore Searching and Virtual Screening
Structure-Based Drug Design - Drugability
Bioinformatics / Chemoinformatics
Systems Biology and biological complexity
Multitarget QSAR
QSPR for novel biomaterials and regenerative medicine
In silico PhysChem Profiling and ADMET
Predictive Toxicology and Risk Assessment - Environmental QSAR
Computational Strategies in Agricultural Research
Novel QSAR Approaches

Contact:
Congress Secretariat
Mr. Gerasimos Kouloumpis
Zita Congress & Travel
Email: gerasimos.kouloumpis@zita-congress.gr

Organised by:
Hellenic Society of Medicinal Chemistry (Greece)

SUMMER SCHOOL ON PHARMACEUTICAL ANALYSIS (SSPA)

Date: June 13-16, 2010
Place: Rimini, Italy

Website:
http://www.scpaweb.org/

The Summer School on Pharmaceutical Analysis (SSPA) is yearly planned under the auspices of the Division of Medicinal Chemistry of the Italian Chemical Society and the EFMC (European Federation for Medicinal Chemistry). This three days school is mainly addressed to researchers and PhD students of the Faculties of Pharmacy and Sciences and to young scientists from pharmaceutical industries.

SSPA is organized on a three-year program on the most advanced analytical methodologies involved into the various stages of the launch of new drugs, from drug discovery (hit selection, structure properties relationship), through drug development (ADME/PK properties, biomarkers discovery) up to formulation and quality control.


Contact person:
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Email: vincenza.andrisano@unibo.it
9TH SWISS COURSE ON MEDICINAL CHEMISTRY

Date: October 10-15, 2010
Place: Leysin, Switzerland
Website: http://www.swiss-chem-soc.ch/smc/leysin/leysin.html

The objectives of the course are to give synthetic chemists, physicochemists, biochemists and pharmacologists a broad and balanced introduction to the background, concepts and tools of medicinal chemistry, a science at the interface of synthetic chemistry, physicochemistry, phytochemistry, biochemistry, pharmacology and toxicology, drug metabolism and disposition, molecular modeling and informatics.

Modern preclinical drug research is thus the focus of the course, which combines dense lectures, tutorials and case studies presented by experts from university and industry. Active participation is encouraged.

Contact person: Prof. Dr. Beat Ernst
Tel: +41 61 267 15 50
Fax: +39-0722-3033-13
Email: Gabi.Lichtenhahn@unibas.ch

THE 19TH LEIDEN/AMSTERDAM CENTER FOR DRUG RESEARCH SCHOOL ON MEDICINAL CHEMISTRY

Date: 19-22 October, 2010
Place: Oegstgeest, The Netherlands
Website: http://www.lacdr.nl/events/19th-school-on-medicinal-chemistry

The School encompasses basic and advanced aspects of drug design, pharmacology and toxicology to provide research chemists in the pharmaceutical industry with the appropriate background for their daily practice. The course provides a thorough introduction in pharmacodynamics, pharmacokinetics and toxicology (ADME-Tox). The impact of molecular biology, genomics and molecular modeling on drug research are also discussed. Newly introduced to the course are cheminformatics and fragment-based design approaches.

In addition, two case histories will give a flavour of chance and strategy in drug development. Speakers come from both pharmaceutical industries and academic research institutes; they have been selected for their scientific expertise as well as didactic qualities.

Contact: Ms. Bea Dekker
Email: bdekker@lacdr.leidenuniv.nl

4TH INTERNATIONAL SYMPOSIUM IN ADVANCES IN SYNTHETIC MEDICINAL CHEMISTRY (ASMC)

To be announced.

FRONTIERS IN MEDICINAL CHEMISTRY: “EMERGING TARGETS, NOVEL CANDIDATES AND INNOVATIVE STRATEGIES”

Date: June 19-21, 2011, Stockholm, Sweden