The official EFMC e-newsletter

MedChem Watch

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The European Federation for Medicinal Chemistry (EFMC) is an independent association founded in 1970 representing 25 Societies from 23 European Countries and more than 6500 Medicinal Chemists. The mission of the EFMC is to advance the science of medicinal chemistry, by promoting cooperation and networking, providing training and mentoring, rewarding scientific excellence and by facilitating communication and influencing stakeholders.

EDITORIAL

Dear colleagues,

this is the last issue of MedChemWatch for this year 2013, a year which has brought some important news in the EFMC organization. First of all, during the Council Meeting, held in Brussels on August 31, Prof. Koen Augustyns has been elected new President of the EFMC for the 2015-2017 term. Koen will start as President Elect by January, 2014. On the same election, prof. Pascal George has been elected as a new EC member, effective from January 2014. Prof. Gerhard Ecker is finishing his service as Past-President, and is leaving the Executive Committee after many years of deep dedication to EFMC. Gerhard has been member, secretary and President of the EC of the EFMC, and among the many initiatives he has sponsored during the years, I would like to mention that he was the founding editor of this newsletter. I am sure to speak for everyone to thank Gerhard for his commitment and in wishing him all the best for his scientific activity.

Another important outcome of the this year's activity is the reshape of the organizational settings of the EFMC. In one of the forthcoming issues, the President will describe in details the news. We can just anticipate here that there will be a lot of opportunity to collaborate for those who are willing to.

In this issue of the newsletter, we continue presenting the European centers for screening, being this time the turn of the Swiss Academic Initiative. We also publish a report on a workshop dedicated to the memory of Prof. Nauta, one of the founding father of the organization and a visionary scientist in the field of GPCR pharmacochemistry.

My best regards,
Gabriele Costantino, *Editor of MedChemWatch*

From the Biomolecular Screening Facility at the EPFL to the Chemical Biology Screening Platform for Switzerland

BY GERARDO TURCATTI

The EPFL-Biomolecular Screening Facility

The Biomolecular Screening Facility (BSF) is an EPFL-founded multidisciplinary laboratory created in 2006 for performing high throughput screening in life sciences-related projects. The platform conceived with a long-term vision was constructed following a development plan according to the broad range of research environment needs rather than to privilege a particular biological discipline or therapeutic area. Therefore, over the years, the BSF has been performing screening campaigns in the major fields (but not limited) of Cancer Research [1-2], Neurobiology [3-4] and Infectious Diseases [5] for researchers interested in Drug Discovery, Chemical Biology and Systems Biology. Our 'generic' and flexible model in terms of field of applications has also been extended and is reflected by the variety of assays proposed and diversity of available compounds collections. Briefly, the BSF performs a variety of assays in 96 and 384 well plate format for in vitro biochemical target-based and cellular assays including image-based phenotypic screens (High Content Screening).using libraries of synthetic chemicals, natural products and synthetic RNA duplexes (siRNAs) for gene known-down assays.

Developing the screening platform

After validating the platform by delivering results from screening campaigns from the local EPFL and associated environment, it has been planned and expected a natural extension of our activities through the interaction with country wide networks, initiatives or national programs. Early on, in 2007, a first development in this direction was possible thanks to the integration of the BSF platform in the Swiss Initiative for Systems Biology (**http://www.systemsx.ch**/) that allowed the platform to specialize in large-scale gene knock-down screens using whole genome siRNAs collections principally through informative screening by imaging assays [6-8]. A more recent critical development is in the frame of the National Centre of Competences in Research (NCCR)-Chemical Biology leaded by the University of Geneva and the EPFL (**http://www.nccr-chembio.ch**/). In this context, the BSF is hosting 'ACCESS', An Academic Chemical Screening Platform for Switzerland.

The NCCR for Chemical Biology

The National Centre of Competence in Research (NCCR) «Chemical Biology – Visualisation and Control of Biological Processes Using Chemistry» has as a main mission to use chemistry tools to obtain a better understanding of life at the molecular level [9]. Until now, few technologies could characterize in detail the countless biochemical activities that constitute a living cell. In the NCCR Chemical Biology, chemists, biochemists, physicists and cell biologists develop innovative techniques based on small molecules and proteins to obtain new information about cellular processes and control them *in situ*. The new tools will be applicable to various biological phenomena like visualizing the activity of selected proteins during cell division and investigating how membranes control the activity of proteins in them. The NCCR is also engaged in establishing a platform (ACCESS) for chemical screening aimed at developing a new generation of molecules with biological effects.

ACCESS

It is therefore one of the goals of this NCCR to establish a platform that provides the scientific community in Switzerland with chemical diversity, screening facilities and know-how in chemical genetics. ACCESS, the platform for Academic Chemical Screens in Switzerland centralized at the EPFL-BSF is becoming a focal point of this NCCR and should permit the Swiss scientific community to profit from the enormous possibilities of chemical biology.

The BSF actively participated in the preparation of this NCCR project and in particular for elaborating the plan for further developing the existing platform in a national specialized center for chemical screens. The main objectives and developments carried out during the first three years of this NCCR are described as follows:

– Increasing the available chemical diversity at the BSF; building the ACCESS chemical collection (link to poster presentation: **http://www.nccr-chembio.ch/fileadmin/user_upload/presentations/posters/**)

– Develop and implement a strategy for collecting compounds from academic organic chemistry labs: The Swiss Chemical collection (link to poster presentation: **http://www.nccr-chembio.ch/fileadmin/user_upload/presentations/posters/ACCESS_Gibelin_Lopez_van-Deursen_Bueno_Banfi_Turcatti.pdf**)

– Definition and validation of the compound management instrumental infrastructure and standard operating procedures for handling and controlling the chemical integrity of chemicals.

Opening an ACCESS antenna at the University of Geneva with selected screening instrumentation including an automated screening microscope for allowing faster progression of in house projects .

Performing chemical screens for the NCCR-Chem Biol partners and moving forward with pilot NCCR-Chem Biol projects towards lead optimization.

Opening the access of the platform to Swiss academic and non profit-research institutions

The ACCESS chemical collection is reaching 100'000 compounds

Thanks to an important instrumental infrastructure, the BSF has been performing screenings since 2006 and handling collections of 130'000 siRNAs and 65'000 chemical compounds. About 15'000 of these small molecules have been available for screening by the whole community of our researchers while a higher proportion of these collections (50'000 compounds, mostly GPCRs and Kinase-targeted libraries) were handled by the platform for few projects due to specific partnering agreements between the research groups and the suppliers of these focused chemical libraries. The BSF 'generic set' of 15'440 chemicals available to every screening project was essentially composed of the Hit-Finder collection (**http://www.maybridge.com/**) of 14,400 compounds, representing the drug-like diversity and the NINDS II collection (**http://www.msdiscovery.com/spectrum.html**) of 1040 bioactive compounds. For providing access to our users to a larger chemical diversity we built up on the previous BSF existing collections by designing, selecting and purchasing different sets or subcollections as described in Table I.

Name of the set	Number of compounds	Suppliers	Comments and status
The Chemically diverse set (or the Lead-like library)	54'000	Enamine Chemdiv Life Chemicals	Commercially available chemical space covered with an average redundancy of six compounds per cluster. The collection was designed using shape as one of the chemical descriptors resulting in a diverse collection enriched with 3D structures and sp3 centers (Figure 1).
Protein-protein interaction (PPi)	5'441	Life Chemicals	This set is composed of compounds chosen by PPi-Machine-Learning-Method (895) and PPi-Rule-of-four (4546)
Natural products (NPs)	2'654	Analyticon, InterBioscreen	These compounds are purified organic molecules from fractionated extracts of two sources, plants and bacteria.
The Pretwick Chemical library (PCL)	1'280	Prestwick Chemicals	A set of known bioactive molecules, approved drugs
Kinases inhibitors	192	Selleckchem	These selected set is composed of 192 kinases inhibitors.
The Natural-products-inspired set	About 15'000	Various suppliers	Currently in progress. Design and selection of a collection of synthetic molecules using all commercially available NPs and derivatives as reference.

Table I: **The ACCESS chemical collection stored at the BSF (by October 2013)**

Collecting compounds from academic labs and establishing compound management procedures

One of the goals of ACCESS is the creation of a screening library with chemical compounds collected from Swiss academic labs. Within the NCCR Chemical Biology, the Biomolecular Screening Facility (BSF) will be hosting and managing this Swiss National Chemical Collection. The strategy for collecting chemicals has been defined and pilot tests have been performed with members of the NCCR that donated the first set of chemical compounds from their labs. We validated our strategic approach for collecting chemical compounds from Swiss organic chemistry academic labs and we established standard operating procedures (SOP) and guidelines for proper handling, transfer and tracking of donated compounds. The diagram described in Figure 2 briefly summarizes these procedures including some aspects of the global compound management strategy.

A successful pilot screening campaign

One of the first screenings performed in the context of the NCCR Chemical Biology has been used by ACCESS as a pilot screening exercise for the multiple validations performed with the new instrumental infrastructure (Figure 3), new implemented procedures and expanded chemical diversity.

The primary assay for this screen aiming at discovering inhibitors of the enzyme Sepiapterin Reductase (SPR) was an in vitro enzymatic assay using a HTRF read-out. The rational approach from the team of Professor Kai Johnsson came from previous research showing that blocking the activity of SPR affects the levels of an important molecule called tetrahydrobiopterin (BH4) in cells. BH4 is critical for the production of neurotransmitters like serotonin and dopamine, and BH4 deficiency causes similar neurological problems to those associated with sulfonamide side effects.

Thanks to the initial ACCESS screening of the collection of known drugs (The Prestwick Chemical Library) and subsequent validations, the group of Kai Johnsson at the EPFL showed for the first time that sulphonamides actually bind to the part of the enzyme that makes BH4. The group's work shows for the first time that sulphonamides interfere with the biosynthesis of neurotransmitters, which can account for their reported neurological side effects. It also helps us understand how the activity of these drugs relates to their molecular structure, and suggests ways of improving their clinical use 10.

This project that screened for the first time the set of the ACCESS diverse collection of 54'000 compounds is currently in the step of validation of expanded chemical structures from validated hits using secondary cellular assays and is progressing towards valuable hits to leads research. The outcome of this and other screening campaigns performed so far is starting to deliver useful information for assessing the value and the quality of the collections we designed at our academic platform for discovering new bioactive chemical entities in Chemical Biology or drug discovery projects.

Opening the platform to Swiss res

In the current phase of opening the ACCESS-BSF platform to other Swiss Academic Institutions, the NCCR Chemical Biology is launching (from October 15, 2013) a call for high impact chemical screening proposals within Switzerland. \(**http://www.nccr-chembio.ch/news-events/news-article/article/call-for-screening-proposals/**)

After project evaluation by the ACCESS steering committee, the management board of the NCCR will sponsor the selected projects entering the platform. The selection procedure will be based on Chemical Biology scientific relevance and feasibility for adapting the proposed validated biochemical or biological assay to a high throughput screening format.

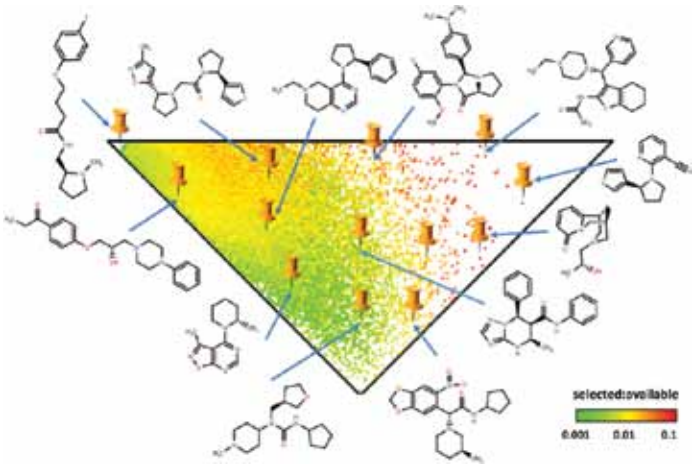

Figure 1. **Density map of the 54'000 compounds of the ACCESS chemical diverse collection**
It has been suggested that "escape from flatland" 11 is beneficial for clinical success of compounds in the drug discovery pipeline. The design of a Diverse Screening Collection for Chemical Biology included molecular shape as a descriptor resulting in an enrichment of three-dimensional molecules.

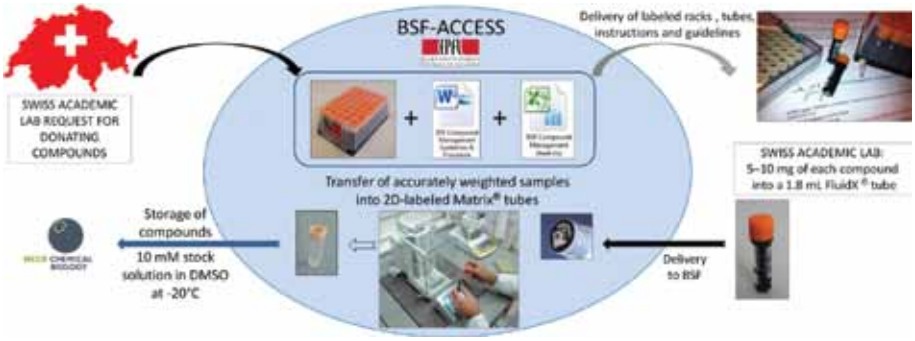

Figure 2: **Global process for collecting synthetic compounds from academic groups**

Figure 3: A) **Compound management using an automated storage system.** Compounds dissolved at 10 mM in DMSO in 2D-bar coded capped tubes (300 uL) are stored at -20°C in an automated store under a controlled low humidity. Plated compounds are also stored in the system using sealed and 1D coded 384 well plates. Compounds tracking and inventory is performed by using a BSF developed Laboratory Information Management System (LIMS).

Figure 3 B) **Checking the chemical integrity of chemical compounds using an UHPLC-MS system**
To estimate the purity of the whole collection in a reasonable time frame, an ultra high performance liquid chromatography system connected to different detectors (Mass spectrometer, UV and CAD) has been installed and the workflow from data acquisition to data processing has been validated. Hits from screens will be systematically analyzed and it is planned to randomly analyze the whole ACCESS collections according to the throughput detrmined.

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Nauta and G Protein-Coupled Receptorology in The Netherlands; a symposium report

BY HENK TIMMERMAN

Professor Wijbe Th. Nauta

Till the sixties of the previous century receptors were a mere concept, a metaphor: a lock with fitting keys, agonists and antagonists. In The Netherlands the pharmacologist Ariëns (Nijmegen) studied properties of the unknown receptors, introduced concepts like intrinsic activity and partial agonism "without knowing"- as he admitted- anything about the nature of receptors at all". In Amsterdam (VU University) the (pharmaco)chemist Nauta was especially interested in the keys, ligands of the receptors. Wijbe Nauta who had selected the histaminergic systems for his research on receptors, has been very instrumental for the acceptance of medicinal chemistry as an independent chemical discipline, but he had good reasons to prefer the term *pharmacochemisty* over medicinal chemistry though. He played a major role in starting the section Pharmacochemistry of the Royal Netherlands Chemical Society and was one of the founders of the European Federation for Medicinal Chemistry, EFMC.

One of the most prominent results of Nauta's investigations of histaminergic (H1) ligands was his proposition that receptors might be proteins in a helix shape. The paper on this idea- there was not any proof - is likely the first one in which the receptor is considered to be a protein, an idea which later on showed to be quite correct.

After the death of Wijbe Nauta (1913- 1986) the *"Nauta Foundation"* was created. This foundation finances since 1992 the in the mean time prestigious Nauta Award of the EFMC (every second year), advanced courses in the field and an extraordinary chair (med. chem.) at the VU University. To mark the 100th anniversary of the birthday of its name giver the foundation and the Division Medicinal Chemistry of the VU University organized on 24-25 June 2013 a symposium in Amsterdam. Awardees of the priz(AW), course organizers (CO) presented inspiring lectures on medicinal chemistry as an interdisciplinary, integrated science: perspectives with a bit of history and nostalgia. The symposium was the stage of the first scientific meeting of the COST Action Glisten (CM1207) a European scientific network in the area of G-protein coupled receptors, GPCRs. Prominent GPCR

researchers showed how new insights in GPCR structures can be used to discover new biologically active ligands and to improve the understanding of the physiological function of these "*fertilizers of medicinal chemistry*".

The Nauta session at the first day of the symposium were chaired by Povl Krogsgard Laarsen and Robin Ganellin, both awardee of the prize. (AW and CO!) presented his views on chances and challenges for medicinal chemists were discussed. Some of these challenges include consideration of the biochemistry of drug metabolism (Bernard Testa, AW) and (epi)genetic control of drug treatment efficacy (Magnus Ingelman-Sundberg, CO). The successful discovery of a CFTR potentiator for the treatment of cystic fibrosis (Peter Grootenhuis, CO) illustrated the potential impact of medicinal chemistry. The scientific progress in G-protein coupled receptor (GPCR) research through the ages (Alex Levitzki, AW) as fertilizers of medicinal chemistry was illustrated by the design and synthesis of ligands that target spinal MOPR-mGluR5 heteromers for the treatment of intractable inflammatory pain (Philip Portoghese, AW), the design and synthesis of diverse histamine H_4 ligands to increase understanding of GPCR-ligand interactions (Eric Haaksma, Nauta chair), and the development of ligands to validate the role of receptors for long chain fatty acids in the treatment of type II diabetes (Graeme Milligan, CO). Medicinal chemistry can play an important role in the deorphanization of GPCRs (Hans Bräuner-Osborne), and the experimental and virtual screening for small, fragment-like GPCR ligands (Gyorgy Keserü), and investigation of allosteric GPCR modulation (Nuska Tschammer) are interesting new research areas. The highly successful meeting was attended by over 100 scientists, and included a speakers' dinner in a famous old house (Felix Meritis) at one of the canals in Amsterdam. At the dinner Gert Folkerts (CO) presented an intriguing speech on "reproducibility in science".

Several other new breakthroughs in GPCR research were covered on the second day of the symposium, including computational approaches to discover new GPCR ligands. The speakers showed how *in silico* approaches can be developed to predict GPCR-ligand interactions (Chris de Graaf), to identify selective ligands from docking to GPCR x-ray structures and homology models (Peter Kolb), and to give new insights into the molecular determinants of GPCR ligand promiscuity (Masha Niv). In combination with the developments in GPCR structural biology, computational tools offer new approaches for GPCR modulation (Leonardo Pardo) and are part of the new wave in GPCR structure-based drug design (Jonathan Mason). The final session showed how the new GPCR structures, crystallized by novel nanobodies (Jan Steyaert), thermostabilizing mutations (Chris Tate), and fusion protein technologies, increase our understanding of GPCR function, ligand efficacy, and receptor activation. Interestingly, the symposium provided the first glimpse of the first crystal structures of the transmembrane domain of class B GPCRs, the glucagon receptor (De Graaf, Katritch) and corticotropin-releasing factor receptor 1 (Mason). The new era of GPCR structural biology enables the identification of molecular signatures of GPCRs (Gebhard Schertler) that offer structural insights into the function and pharmacology of the GPCR superfamily (Vsevolod (Seva) Katritch).

For more informations please see also:
www. Nautastichting.nl
www. Medchemsymposium.org
www. Glisten-gpcr.eu

Chris de Graaf

Most meritorious runner up of the EFMC Prize for a Young Researcher in Academia 2012 and 2013

BY CHRIS DE GRAAF

In silico veritas: Medicinal chemistry through the 3D looking glass

My interest in investigating the structure and function of pharmacologically relevant protein systems originates from my study Chemistry at the University of Amsterdam (1997-2002). The drive to perform scientific research and study the molecular determinants of protein-ligand interactions aligned with an interesting PhD position in the field of computational medicinal chemistry and toxicology at VU University Amsterdam. My PhD project (under the supervision of Prof. Nico Vermeulen) was part of a multidisciplinary research program that combined computational chemistry, organic chemistry, biochemistry, spectroscopy, and molecular toxicology. From 2002 to 2006 I developed complementary computational approaches to study ligand binding to cytochrome P450 enzymes, and experienced the challenges, strengths, and joys of working in an interdisciplinary research team (in particular with my scientific "P450 partner in crime" Dr. Peter Keizers). I furthermore learned about the power of international scientific collaboration during gratifying research internships in the groups of Prof. Gerd Folkers at ETH-Zurich (to work on molecule docking methods) and Prof. Rebecca Wade at EML Heidelberg/HITS (on advanced molecular dynamics simulation techniques).

Following my PhD, I was eager to further spread my scientific wings and to explore research in a pharmaceutical industry setting. A post-doc position in the Structural Chemogenomics group of Dr. Didier Rognan at the University of Strasbourg in collaboration with AstraZeneca Pharmaceuticals offered me the opportunity to do just that. I was working closely together with scientists from different AstraZeneca R&D sites in the US, UK, and Sweden (including Dr. Ola Engkvist, Dr. Igor Shamovsky, and Dr. Fabrizio Giordanetto), and the computational models and methods I developed were successfully applied in drug development projects to discover and optimize new GPCR ligands. In between the project milestones and work visits to AstraZeneca R&D sites, the stimulating environment in Didier's group offered me the freedom to perform more fundamental scientific studies on the development of new G Protein-coupled receptor modeling and virtual screening techniques. For example, we performed one of the first studies to predict functional selectivity of GPCR ligands using an agonist customized model based on the first antagonists bound crystal structure of a human GPCR (the beta-2 adrenergic receptor)[1] and conducted the first successful structure-based virtual screening study to identify small allosteric modulators of class B GPCRs.[2] During my post-doc abroad, I did not only appreciate *best of both worlds* professionally (academia and industry), but also enjoyed the French joie de vivre with a touch of Alsacian Gründlichkeit: From vélo-tout-terrain trips up the flanks of the Vosges, amidst vineyards and deserted pine forests, towards a rewarding Gewürztraminer-Münster-apéro.

Medicinal Chemistry in Amsterdam: Interdisciplinary scientific teamwork

At the end of 2008, Dr. Iwan de Esch and Prof. Rob Leurs convinced me to join the Division Medicinal Chemistry at VU University Amsterdam to lead the computational medicinal chemistry team as an assistant professor. The Division Medicinal Chemistry (headed by Prof. Rob Leurs) combines computer-aided drug design and chemical synthesis

(Dr. Iwan de Esch, Dr. Maikel Wijtmans, and myself) with molecular pharmacology and biochemistry (Prof. Martine Smit, Dr. Henry Vischer, Dr. Marco Siderius) to understand the molecular details of ligand-receptor interactions, to elucidate receptor signaling networks, and to use this knowledge for the computational design and synthesis of new bioactive molecules. We work on a diverse set of pharmaceutically relevant protein targets, including G protein-coupled receptors (in particular histamine and chemokine receptors), as well as ligand-gated ion channels, kinases, and phosphodiesterases. All are important targets in the development of drugs against for example inflammation, cancer, neuronal disorders, and neglected tropical diseases.

In this interdisciplinary research environment my team and I have developed chemoinformatics tools and modeling protocols that allow explicit incorporation of experimental data and, *vice versa*, are used to steer medicinal chemistry programs. Current methods that we use in our studies include ligand-, protein-, and protein-ligand interaction fingerprint based virtual screening methods (e.g. *EDprints*[3], *FLAP*[4] (with Prof. Gabriele Cruciani, University of Perugia), *IFP*[5] (with Dr. Didier Rognan) *Snooker*[6] (with Prof. Jacob de Vlieg, Netherlands e-Science Center)). In the past years we have furthermore constructed several structural chemogenomics databases to navigate protein-ligand interaction space of kinases (*KLIFS*)[7], PDEs (*PDEStrIAn*), and aminergic GPCRs[8]. My group has built a track record in protein modeling and virtual screening, exemplified by winning an international competition (GPCR DOCK 2010)[9] to predict the three-dimensional coordinates of a ligand bound protein crystal structure (of the CXCR4 chemokine receptor), and by obtaining the highest structure-based virtual screening hit rate to discover novel biologically active molecules (for the histamine H_1 receptor, with Prof. So Iwata (Imperial College)).[5]

Computational chemists can (and, in my opinion, should) play an important role as bridge builders between experimental research disciplines. For most of our medicinal chemists, computer-aided drug design techniques are essential tools to optimize molecules. In our medicinal chemistry group there is no rational ligand design without a pharmacophore or protein-ligand interaction model. Molecular modeling simulations offer insights into protein-ligand interactions at an atomic level. These three-dimensional *in silico* models guide our molecular pharmacologists to probe protein-ligand binding pockets even further with, for example, site-directed mutagenesis studies.[10-11] This iterative multidisciplinary teamwork within the Medicinal Chemistry Divison is highly inspiring.

In 2009 I obtained a prestigious *Veni* Grant from the Netherlands Organization for Scientific Research (NWO) to set up a research line in the computational prediction of protein-ligand interactions. My team has developed and applied new *in silico* methods to discover ligands for various proteins and to predict protein-ligand selectivity in order to design better drugs with fewer side effects.[4-5, 12-14] Together with my colleagues in the Medicinal Chemistry Division at VU University Amsterdam I am currently building a fragment-based chemogenomics platform[14] based on *in-house* experimental fragment screening data, to develop *in silico* modeling techniques to increase our understanding of the molecular details of protein-ligand selectivity. This platform currently contains not only information and models of intended drug targets (including GPCRs, ligand-gated ion channels, kinases, and phosphodiesterases) but also of undesired drug targets (including cytochrome P450 enzymes and hERG). Our fragment-based chemogenomics approach reduces the molecular complexity that is used to probe different protein binding sites to a level that enables the development of innovative computer models to predict selective protein-ligand interactions. The new computer models will be used for the discovery and design of new ligands with specific protein selectivity profiles (*i.e.*, molecules that are able to modulate one specific protein or *multiple* therapeutic proteins simultaneously (polyharmacology) but do *not* interact with off-targets that can cause harmful effects).

These efforts align with the set up of an institutional Chemical Biology platform (under the auspices of our Medicinal Chemistry group) that will link scientific efforts of the *Amsterdam Institute for Molecules, Medicines, and Systems* (AIMMS) and the VU University Medical Center (VUMC). In the past year I have furthermore been involved in setting up European networks to study G protein-coupled receptors (GLISTEN COST Action CM1207, with Dr. Peter Kolb) and to optimize the binding kinetics of drugs (K4DD *Innovative Medicines Initiative* (IMI) consortium). These international networks bring together a wide range of complementary methods and expertise that help us and our collaborators to further strengthen and extend the impact of our scientific research. I recently enjoyed participating in such an integrated international scientific research team with the *Scripps Research Institute* (led by Prof. Ray Stevens), *Shanghai Institute for Materia Medica* (led by Prof. Ming-Wei Wang), and *Novo Nordisk*, which reported the first crystal structure of the transmembrane domain of a class B GPCR (the glucagon receptor), and performed extensive mutagenesis studies that

enabled the construction of a 3D structural model that predicts how glucagon binds its receptor.[15]

I consider *teaching* as a unique and attractive aspect of an academic environment, that is highly complementary to scientific research (and requires at least as much skills and devotion). The many motivated bachelor and master students in our study programs make me eager to learn new things every day. Moreover, I feel privileged to work and have worked with many talented and skilled PhD students and post-docs in the VU computational medicinal chemistry team. I would like to thank all current and former (guest) team players (in particular Albert Kooistra, Luc Roumen, Enade Istyastono, Sabine Schultes, Francesco Sirci, Marijn Sanders, Oscar van Linden, Chimed Jansen, Sebastiaan Kuhne) for their inspiring achievements. These talented young scientists as well as my other (ex-)colleagues and collaborators definitely deserve their fair part of the scientific credits I received as most meritorious runner up for the EFMC Prize for a Young Medicinal Chemist in 2012 and 2013.

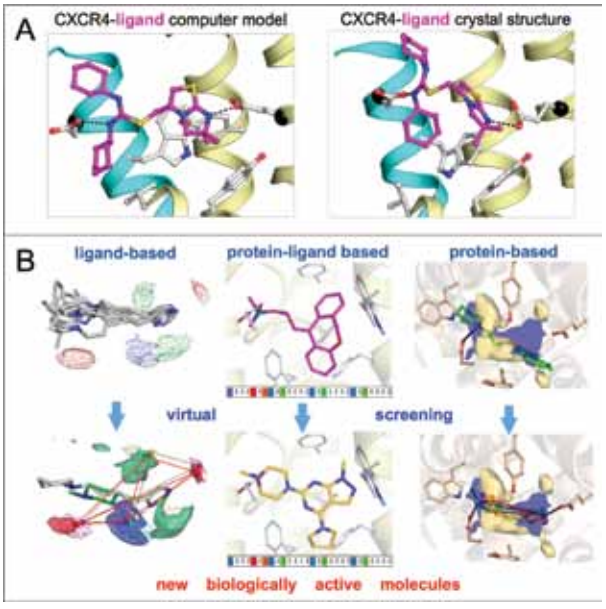

Figure: Examples of the in silico prediction of protein-ligand interactions by the computational medicinal chemistry team of Chris de Graaf: A) In the worldwide GPCR DOCK 2010 competition9 the VU-MedChem team of de Graaf constructed a computational three-dimensional model that correctly predicted the highest number of protein-ligand contacts of all 103 submissions from 25 research groups (prior to release of the experimentally determined CXCR4-ligand co-crystal structure). B) De Graaf and colleagues use ligand-based and protein-based molecular fingerprints for virtual screening of large chemical libraries to discover novel small molecule modulators of pharmaceutically relevant proteins.2,4-5,11-12

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THE EFMC PRIZE

FOR A YOUNG MEDICINAL CHEMIST IN ACADEMIA

To acknowledge and recognize an outstanding young medicinal chemist working in Academia within Europe.

The **Prize** is given annually to a young medicinal chemist (≤ 10 years after PhD), and consists of a diploma, €1.000 and an invitation to give a short presentation at the XXIII EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC), September 7-11, 2014, Lisbon, Portugal.
Two additional nominees will also be identified and acknowledged.

Applications should be done via the application form on www.efmc.info and should consist of:
– a one-page letter by the candidate including a short rationale for their application
– one page with his/her 5 most important publications
– a brief cv of the candidate
– abstract of potential oral presentation

THE EFMC PRIZE

FOR A YOUNG MEDICINAL CHEMIST IN INDUSTRY

To acknowledge and recognize an outstanding young medicinal chemist working in industry within Europe.

The **Prize** is given annually to a young medicinal chemist (≤ 10 years after PhD), and consists of a diploma, €1.000 and an invitation to give a short presentation at the XXIII EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC), September 7-11, 2014, Lisbon, Portugal.
Two additional nominees will also be identified and acknowledged.

Nominations should be submitted by the candidate's supervisor via the submission form on www.efmc.info and should consist of:
– a letter by the supervisor
– a brief cv of the candidate
– abstract of potential oral presentation

Deadline for Nominations is January 31, 2014

EFMC
European Federation
for Medicinal Chemistry

See www.efmc.info for full details.

News from the Societies

BY ERDEN BANOGLU

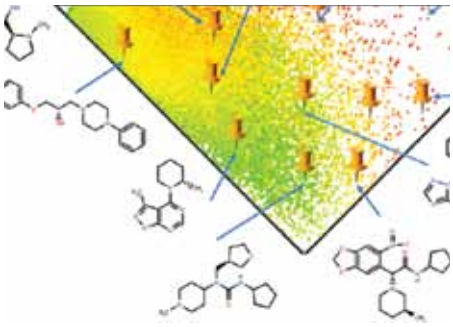
DIVISION OF MEDICINAL CHEMISTRY OF THE ITALIAN CHEMICAL SOCIETY

MEETING REPORT

XXII National Meeting on Medicinal Chemistry

The 22nd edition of the National Meeting on Medicinal Chemistry (XXII NMMC) was organized by the Division of Medicinal Chemistry of the Italian Chemical Society in the Campus of Sapienza University of Rome, Italy, on September 10-13, 2013. The XXII NMMC took place under the patronages of the Italian Chemical Society, European Federation for Medicinal Chemistry (EFMC) and other Italian institutions, and was sponsored by several pharma and related industries. This Meeting aimed to disseminate the results of top quality scientific research, stimulating continuous innovation and international collaborations in the field of the drug chemistry, pharmaceutical technology and food sciences.

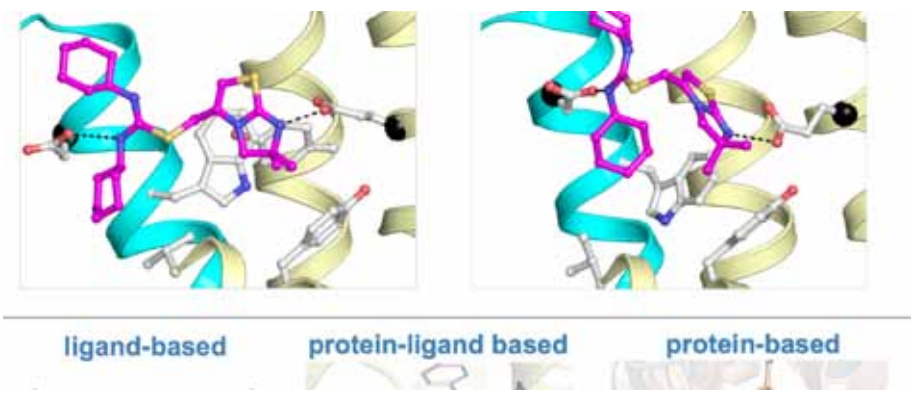
325 registered participants attended the XXII NMMC, whereof 252 (77 %) were Italians; 42 (13%) attendants arrived from other European countries and 23 (7%) were from non-EU countries. The Meeting got 65 (20%) trainees registrations, and 23 (7%) attendants were from industry. The XXII NMMC covered a number of topics of leading research areas, namely Oncology and Epigenetics, Inflammatory, Metabolic and Cardiovascular Diseases, Analytical Tools in Drug Discovery and Development, Infectious



Diseases and Drug Resistance, Natural Products and Nutraceuticals, Computational Science in Drug Discovery, New Approaches in Drug Discovery and CNS Diseases. In summary, the XXII NMMC provided 69 lectures covering 8 topics and 128 posters over 2 poster sessions. 12 selected short communications were supported by the Italian Division of Medicinal Chemistry as a part of the young scientists support program.

The venue on September 10 was located at the Aula Magna room of Campus Sapienza. The XXII NMMC opening ceremony started with the greetings of the Rector of Sapienza University Luigi Frati. After the Farmindustria and Musaio Awards, the Meeting began with the opening lecture led by Dario Neri (ETH, Zurich; Armed antibodies and targeted cytotoxics: from the bench to the clinic) and the plenary lecture (P) by Uli Stilz (Sanofi-Aventis, Frankfurt a.M.; Cross talk between small molecules and biological systems: potential for systems medicine in industry) as the President of EFMC. The opening session followed by welcome dinner at the terrace behind the Aula Magna room.

On days 2 to 4 the activities of the XXII NMMC were then hosted by Department of Drug Chemistry and Technologies. On September 11 (day 2) the program began with the P led by Stefan Laufer (EK University, Tübingen; Next generation protein kinase inhibitors: When selectivity counts) After this P, the meeting program split into two parallel oral sessions. The first session on Oncology and Epigenetics provided keynote (K) lectures led by Andrew Westwell (Cardiff University, UK) and Claudiu Supuran (University of Firenze), while the parallel session Inflammatory,



Metabolic and Cardiovascular Diseases started on with the K by Marcello Allegretti (Dompè). The afternoon session showed the Ks led by Takayoshi Suzuki (Kyoto Prefectural University of Medicine, Japan) and Gianluca Sbardella (University of Salerno) of Oncology and Epigenetics, and the Ks by Klaus Wanner (Ludwig-Maximilians University, Munich) and Federico Riccardi Sirtori (Nerviano Medical Sciences, Nerviano) of Analytical Tools in Drug Discovery and Development. Poster session I on September 11 exhibited 66 posters of these topics. On September 12 (day 3) the program began with the P performed by Anna Tramontano (Sapienza University, Roma; The computational analysis of biomolecular interactions and its potential impact on drug discovery). Infectious Diseases and Drug Resistance showed Ks managed by Chris Meier (University of Hamburg), Robert Bates (GlaxoSmithKline, Madrid), and Andrea Brancale (Cardiff University), while the parallel sessions Natural Products and Nutraceuticals and Computational Sciences in Drug Discovery had Ks led by Fulvio Mattivi (Edmund Mach Foundation, S.M. all'Adige) and Ashraf Virmani (Sigma-Tau, Pomezia) and Andrea Cavalli (University of Bologna), respectively. Poster session II September 12 exhibited 62 posters including topics of days 3 and 4. On September 13 (day 4) Adrian Ijzerman (Leiden University) held the P (A case for G protein-peopled receptors). The following sessions were New Approaches in Drug Discovery with the Ks led by Enrico Stura (CEA, Division of Life Sciences) and Daniel Rauh (Technische Universität Dortmund), and CNS Diseases, with Ks byFerdinando Nicoletti (Sapienza University of Roma) an Piero A. Salvadori (CNR of Pisa).

The XXII NMMC was successfully completed. The participants highly appreciated the qualities of the speakers and careful organization. During the meeting, continued effort to ensure quality of scientificresearch was impressive. This meeting has been a good forum to exchange experiences and establish promising working collaborations in the areas of pharmaceutical, technological and food sciences.

THE BIOLOGICAL AND MEDICINAL CHEMISTRY SECTOR (BMCS) OF THE ROYAL SOCIETY OF CHEMISTRY (RSC)

The Malcolm Campbell Memorial Award is awarded biennially by the RSC BMCS to commemorate Professor Campbell's outstanding contributions in a broad range of chemistry and their applications to the understanding of bioactivity. The award comprises £2000 and a medal and this year was awarded to the team at AstraZeneca for work involved in the discovery of BrilintaTM/BriliqueTM. This was presented to the winning team at the RSC/SCI Medicinal Chemistry Symposium on 10th September by the local Member of Parliament Julian Huppert. Garry Pairaudeau accepted the award on behalf of the other team members who were Dave Chapman, John Dixon, Simon Guile and Bob Humphries

See http://www.rsc.org/Membership/Networking/InterestGroups/BMCS/index.asp for more info

The AZ Team

Prize presentation

EFMC Short Course

8th EFMC Short Course on Medicinal Chemistry

ENGINEERING OF BIOPHARMACEUTICALS

March 16-19, 2014
Oegstgeest, near Leiden, The Netherlands

This intensive course is intended for scientists with interests in the field of peptide and protein engineering covering interesting topics around synthetic peptides, engineered proteins and therapeutic antibodies. The number of participants will be limited to 35 to assure the possibility for in-depth discussions. The presentations and tutorials will be given by academic and industrial experts in the various topics and will cover broad historical perspectives and in depth details of important engineering technologies. The presenters will also include interesting applications as well as future aspects in an informal approach aiming for high level of interaction of the participants.

Course Outline

The development of future biopharmaceuticals will depend on research at the interfaces between several scientific disciplines including organic chemistry, physical chemistry, biophysics, protein chemistry and molecular biology. The interplay between these fields will have a key role for improving our molecular understanding of peptides and proteins and thus for developing future drug candidates.

This course will focus on strategies on how to design and engineer biopharmaceuticals and will provide participants with insight to this important field of bioscience, which are applicable in academic and pharmaceutical contexts.

The course will cover several fundamental aspects of peptide chemistry methodologies, selective modifications of proteins, ligation chemistries and regioselective coupling reactions. The biophysical characterization of peptide and proteins will be integrated in the lectures. The course will also cover various methods of semi-synthetic and synthetic modifications of proteins with focus on the application to drug discovery. Finally the course will give an insight to therapeutic antibodies including screening, optimization an engineering aspects. Thus, various issues of development of biopharmaceuticals as well as discussions of different strategies to improve peptide and protein properties to biopharmaceuticals will be the primary focus of the course.

Course Organisers
Jesper LAU
Novo Nordisk, DK

Local Organiser
Henk Timmerman
VU University Amsterdam, NL

Deadline for preregistration
February 17, 2014

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

Fee
€ 1.675,00
Including accommodation, breakfast, coffee breaks, lunches and dinners during the days of the conference

Contact
EFMC Administrative Secretariat
LD Organisation sprl
Scientific Conference Producers
Rue Michel de Ghelderode 33/2
1348 Louvain-la-Neuve, Belgium
Tel: +32 10 45 47 74 Fax: +32 10 45 97 19
Mail: administration@efmc.info
Web: www.efmcshortcourses.org

EUROPEAN FEDERATION FOR MEDICINAL CHEMISTRY

EFMC NEWS

BY NELE COULIER AND KOEN AUGUSTYNS

The **5th edition of the International Symposium on Advances in Medicinal Chemistry (ASMC 2013)** took place in Moscow, Russia on May 5-8, 2013. Prof. Peter Seeberger (Max Planck Institute of Colloids and Interfaces, DE) and Dr Alan Palkowitz (Eli Lilly & Company, USA) were the chairmen of the symposium, where American and European chemists met Eastern European scientists in the areas of synthetic and medicinal chemistry. The symposium, organised by EFMC and ChemBridge Corporation attracted 235 participants representing a large number of countries, pharmaceutical and biotechnology companies and academic institutions. The next edition of the symposium will take place in Kiev, Ukraine on May 3-7, 2015.

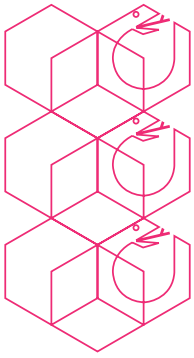
Together with the American Chemical Society (ACS), EFMC organized the **Frontiers in Medicinal Chemistry Meeting**, which took place in San Francisco on June 23-26, 2013. This symposium is the fourth in the series initiated in Siena, Italy in 2007 and continued in Barcelona, Spain in 2009 and Stockholm, Sweden in 2011. The theme of this year's meeting was "Emerging Targets, Novel Candidates and Innovative Strategies, and with 288 participants, the 2013 edition was a big success! The next edition will be held in 2015 in Europe.

For 2014, EFMC and the Group of Medicinal Chemistry of the Portuguese Chemical Society are preparing the **XXIII EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC)**, scheduled to be held on September 7-11, 2014 in Lisbon, Portugal. The 2014 edition will continue the tradition established by these biennial symposia and will cover drug discovery advances in the major therapeutic areas, including neglected diseases, CNS disorders, inflammation, metabolic disorders, and oncology. EFMC-ISMC 2014 will present the most recent advances in lead identification and optimization strategies, drug design and profiling technologies, and illustrate the impact of biomarkers and imaging at the interfaces between chemistry, biology and experimental medicine. Particular emphasis will be put on first time disclosures, recent highlights in medicinal chemistry, and organic synthesis which had a strong impact on medicinal chemistry. Online registration and abstract submission are now open! All info is available on the website **www.efmc-ismc.org**

To create a network of young European investigators in Medicinal Chemistry, to stimulate young European investigators in Medicinal Chemistry to share their scientific work with peers and inspiring leaders in the field, and to create competition and excellence in Medicinal Chemistry within Europe, the EFMC decided to organize a **Young Medicinal Chemist Symposium** on the Saturday preceding the EFMC-ISMC Symposium. More details will soon be available on the websites **www.efmc.info** and **www.efmc-ismc.org** and young scientists will be encouraged to participate!

At the annual EFMC Council meeting, the Council unanimously elected Prof. Koen Augustyns (University of Antwerp, Belgium), current secretary, as President Elect. His term will start on January 1st 2014, and on January 1st 2015 he will automatically become EFMC President. Phil Jones (UK) has been reelected as EC member for a period of 2 years, and also Pascal George (France) has been elected EC member. Their terms will start on January 1st, 2014.

EFMC NEWS



EFMC 2014 AWARDS

To acknowledge outstanding achievements in the field of Medicinal Chemistry, EFMC is conferring every two years three Awards on the occasion of an International Symposium on Medicinal Chemistry. The 2014 Awards will be conferred on the occasion of the XXIII EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC) to be held in Lisbon, Portugal on September 7-11, 2014.

The EFMC Awards include the Nauta Award for Pharmacochemistry, the UCB-Ehrlich Award for Excellence in Medicinal Chemistry and the Prous Institute-Overton and Meyer Award for New Technologies in Drug Discovery. The three awards consist of a diploma, € 7.500 and an invitation for a lecture by the Award recipient at the upcoming EFMC-ISMC. Deadline for submission is January 31, 2014. Self-nominations are also accepted. Regulations and information on the submission process are available on the EFMC website **www.efmc.info**

THE EFMC PRIZE

To acknowledge and recognize an outstanding young medicinal chemist (≤ 10 years after PhD) working in industry or in academia within Europe, EFMC established the EFMC Prize for a Young Medicinal Chemist in Industry and the EFMC Prize for a Young Medicinal Chemist in Academia. The Prizes consist of a diploma, € 1.000 and an invitation for a short presentation at the upcoming XXIII EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC), scheduled to take place on September 7-11, 2014 in Lisbon, Portugal. Deadline for nominations/applications is January 31, 2014. More information is available on **www.efmc.info**

The publication of the 12th edition of the EFMC Yearbook is scheduled for January 2014. The Yearbook will be distributed electronically to all members of the EFMC database, as well as to the members of the National Adhering Organisations (25 scientific organisations from 23 European countries). In addition, hard copies of the EFMC Yearbook will be distributed at all scientific meetings organised or sponsored by EFMC. If you would like to receive the electronic version of the EFMC Yearbook 2014, we invite you to register via the EFMC website **www.efmc.info**

With the aim to support training and networking within the medicinal chemistry community, EFMC is organising twice a year an EFMC Short Course on Medicinal Chemistry. In March 2014, Dr Jesper Lau (Novo Nordisk, Denmark) will organize the 8th EFMC Short Course on "Engineering of Biopharmaceuticals". This Spring 2014 Short Course is planned for March 16-19, 2014 and will take place in Oegstgeest (near Leiden), The Netherlands. For more information and registration, we refer to the website **www.efmcshortcourses.org**

EFMC EVENTS

BY NELE COULIER AND KOEN AUGUSTYNS

EFMC ORGANISED EVENTS

8th Short Course
on Medicinal Chemistry
March 16-19, 2014
Oestgeest, The Netherlands
www.efmcshortcourses.org

EFMC-ISMC 2014
XXIII International Symposium on Medicinal Chemistry
September 7-11, 2014
Lisbon, Portugal
www.efmc-ismc.org

EFMC SPONSORED EVENTS

SCI Meeting
Towards new Therapeutics for Diseases of the Developing World
May 11-13, 2014
Tres Cantos, Spain

EuroQSAR 2014
20th European Symposium on Quantitative Structure-Activity Relationship
August 31 – September 4, 2014
St. Petersburg, Russia
www.euroqsar2014.org

MedChemComm is delighted to welcome Professor Christa E. Müller (University of Bonn, Germany) as our new Associate Editor for Europe.

Biography
Christa Müller studied pharmacy at the University of Tübingen, Germany, and received her Ph.D. in Pharmaceutical/Medicinal Chemistry from the same university. After a postdoctoral stay with John W. Daly (1989-1990 and 1992) at the Laboratory of Bioorganic Chemistry, National Institutes of Health, in Bethesda, Maryland, USA, she completed her habilitation thesis at the University of Tübingen in 1994, and became Associate Professor of Pharmaceutical Chemistry at Würzburg University in the same year. Since 1998 she is full professor of Pharmaceutical Chemistry at Bonn University. She is a co-founder of the Pharma-Center Bonn (www.pharma-zentrum.uni-bonn.de), and has >250 publications in the field of medicinal chemistry and pharmacology.
Her scientific interests are focused on the medicinal chemistry and molecular pharmacology of purine-binding membrane proteins (purine receptors, ectonucleotidases) and lipid-activated orphan G protein-coupled receptors. Disease indications include neurodegenerative and inflammatory diseases and cancer. Her activities are ranging from basic research to collaborative drug development projects with pharma industry partners.

MedChemComm has what it takes to become a leading journal of Medicinal Chemistry. It fills a gap since it differs from other med chem journals due to its wide scope and its unique format. I'm looking forward to seeing everyone's exciting contributions and support!"

EFMC 2014 AWARDS

Call for nominations

DEADLINE: JANUARY 31, 2014

The awards will be conferred on the occasion of the XXIII EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC), to be held in Lisbon, Portugal, September 7-11, 2014

The Nauta Award for Pharmacochemistry

For the advancement of medicinal chemistry and the development of international organisational structures in Medicinal Chemistry. The Award will be given for outstanding achievements in the field of Medicinal Chemistry.

The UCB-Ehrlich Award for Excellence in Medicinal Chemistry

To acknowledge and recognize outstanding research in the field of Medicinal Chemistry in its broadest sense by a young scientist. This Award has been established with the support of UCB Pharma.

The Prous Institute-Overton and Meyer Award for New Technologies in Drug Discovery

To encourage innovation and investigation in technological development related to drug discovery, this Award established with the support of Prous Institute will be given for the discovery, evaluation or use of new technologies.

Nominations for these Awards consist of a nomination letter, a brief CV, including a list of selected publications and two supporting letters. Self-nominations are also accepted. The nominations should be submitted to the Chairman of the Juries, Dr Hans Ulrich Stilz, President of EFMC, c\o EFMC Administrative Secretariat, Rue Michel de Ghelderode 33/2, 1348, Louvain-la-Neuve, Belgium FAX: +32 10 45 97 19 E-MAIL: awards@efmc.info

Please visit www.efmc.info for more information and Award regulations

EUROPEAN FEDERATION FOR MEDICINAL CHEMISTRY

EFMC | ISMC 2014

XXIII International Symposium on Medicinal Chemistry

Lisbon, Portugal September 7-11, 2014

SESSIONS AND SESSION COORDINATORS

ALLOSTERIC MODULATORS FOR CNS DISEASES
Wolfgang Froestl (AC Immune, CH)

ANTIINFECTIVES: ANTIVIRALS, ANTIBACTERIALS (AFMC SESSION)
Ming-Hua Hsu (National Tsing Hua University, TW)

APPLICATIONS OF POSITRON EMISSION TOMOGRAPHY IN DRUG DISCOVERY (ACS SESSION I)
Sam Bonacorsi (Bristol-Myers Squibb, US)

COMBATING ANTIBIOTIC RESISTANCE
Ada Yonath (Weizmann Institute of Science, IL)

COMPUTATIONAL APPROACHES TO GUIDE MEDICINAL CHEMISTRY
Helmut Grubmüller
(Max Planck Institute for Biophysical Chemistry, DE)

DECODING DISEASE: LIGANDING AND DRUGGING BROMODOMAIN EPIGENETIC READERS
Stuart J. Conway (University of Oxford, UK)

GPCR STRUCTURAL BIOLOGY: NEW THERAPEUTIC OPPORTUNITIES?
Jan Steyaert (VUB – University of Brussels, BE)

INFLAMMATION: THE COMMON LINK IN MULTIFACTORIAL DISORDERS?
Angeliki Kourounakis (University of Athens, GR)

HOT TOPICS IN ION CHANNELS
Brian Cox (Novartis Institutes for Biomedical Research, UK)

NEW STRATEGIES FOR LEAD GENERATION
Maria Blanco-Pillado (Eli Lilly and Company, US)

NEW THERAPIES FOR METABOLIC DISORDERS
Jürgen Mack (Boehringer Ingelheim, DE)

NEURODEGENERATION – DEEPER UNDERSTANDING OF DISEASE BIOLOGY AND EMERGING THERAPEUTIC OPTIONS
Andrew Thomas (F. Hoffmann-La Roche, CH)

NEW CHEMICAL ENTITIES: BEYOND SMALL MOLECULES
Stan Van Boeckel (Leiden Institute of Chemistry, NL)

NOVEL AGENTS FOR THE TREATMENT OF C. DIFFICILE (ACS SESSION II)
Steven Firestine (Wayne State University, US)

ONCOLOGY: KINASES AND BEYOND
Mario Varasi (European Institute of Oncology, IT)

KINETC AND THERMODYNAMIC ASPECTS OF LIGAND BINDING
Gyorgy Keseru (Hungarian Academy of Sciences, HU)

ORGANIC SYNTHESIS THAT CHANGED MEDICINAL CHEMISTRY
Morten Jorgensen (Lundbeck, DK)

ORGANIC SYNTHESIS: NEW DEVELOPMENTS (EUCHEMS SESSION)
Péter Mátyus (Semmelweis University, HU)

MECHANISM-BASED PREDICTION OF DRUG-INDUCED LIVER INJURY (EUFEPS SESSION)
Nico Vermeulen (VU University Amsterdam, NL)

TAMING NATURAL PRODUCTS: NOVEL NATURAL PRODUCTS, COMPLEX SYNTHESIS, MUTASYNTHESIS
Anake Kijjoa (University of Porto, PT)

TRANSLATIONAL MEDICINE: CASE STUDIES WITH BIOMARKERS AND PKPD MODELING
Yves Auberson (Novartis Institute for Biomedical Research, CH)

NEGLECTED TROPICAL DISEASES: SHAPING FUTURE TRENDS
Kelly Chibale (University of Cape Town, ZA)

FIRST TIME DISCLOSURERS
Laurence Lafanechère (CNRS, FR)

RECENT HIGHLIGHTS IN MEDICINAL CHEMISTRY
Carlos Montanari (University of Sao Paulo, BR)

CONFIRMED PLENARY LECTURES

Chas BOUNTRA
(University of Oxford, UK)
Karin BRINER
(Novartis, US)
Aaron CIECHANOVER
(Technion-Israel Institute of Technology, IL)
Ismail KOLA
(UCB, BE)

EFMC
European Federation for Medicinal Chemistry

Sociedade Portuguesa de Química

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

- Prize for a Young Medicinal Chemist in Industry
- Prize for a Young Medicinal Chemist in Academia

OTHER PRIZE LECTURES

- IUPAC-Richter Prize in Medicinal Chemistry
- MedChemComm Lectureship

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