

Dear Colleague

The year 2009 has been a quite exciting one for EFMC and for Medicinal Chemistry in general. We faced a lot of challenges and several important decisions had to be made. First of all, the year started with hiring Nele Coulier as part time secretary working in the office of Ly Differding in Brussels. Nele gives not only great support to Koen, Rasmus and me in our daily tasks, but finally supports all of us by creating a sustainable infrastructure for EFMC.

Due to the global financial crisis, the year 2009 was economically extremely difficult, and a lot of meetings had to be cancelled or made a loss. It is thus a pleasure for me to inform you that all events EFMC was involved in were a success. In March I had the honour to open the first EFMC Short Course – Improving Compound Quality: Physical Chemistry and DMPK Properties in Drug Discovery. Principles, Assays and Predictions. The Course took place in Oegstgeest, The Netherlands, and was fully booked. We received a lot of positive feedback and I am very grateful to Peter Matyus, the chair of the Education and Training Committee, and to Henk Timmerman and Han van de Waterbeemd, who organised the course. The second EFMC Short Course will focus on Safety and Attrition and will be organised again in Oegstgeest from April 11-14. This intensive course is intended for scientists working in the field and the presentations will be given by senior scientists both from industry and academia. The number of participants will be limited to 35, to favour in depth discussion. Should the number of applications exceed the maximum, preference will be given to applicants from EFMC adhering countries and employees of EFMC corporate members.

In August the third edition of the International Symposium on Advances in Synthetic and Medicinal Chemistry (ASMC), jointly organised by ChemBridge Corporation and EFMC and supported by the ACS Division of Medicinal Chemistry, took place in Kiev, Ukraine. Although this time “only” about 350 scientists attended the meeting, it still was a big success, both scientifically and also financially. The successful outcome of this meeting, which represents a unique flair of covering hot topics from organic and medicinal chemistry, is definitely due to the top quality programme put together by the two chairs of the meeting, Scott Biller (Novartis) and Eric Carreira (ETH Zuerich). Without their invaluable contributions, the enthusiasm of Edmond Differding (UCB), Gene Vaisberg, Sergey Altshteyn (ChemBridge Corporation), Andrey Tolmachev and Aleksander Kostyuk (Enamine) as well as the perfect organisation of the event by Ly Differding and her team, this meeting would not have been possible. I also want to thank the members of the International Scientific Committee for all their contributions. The next meeting will take place in 2011 in Moscow, the city where this successful series started in 2004.

Finally, in October EFMC and the Sociedad Espanola de Quimica Terapeutica organised the second edition of Frontiers in Medicinal Chemistry in the wonderful city of Barcelona. This meeting is unique in its setting, as half of the speakers are nominated by the hosting country and the other 50% are complemented by the EFMC. This time, the meeting was organised under the topic “Emerging Targets, Novel Candidates and Innovative Strategies”. The symposium was overbooked and we had to close the registration two months ahead of the event. I want to take the occasion to

sincerely thank Maria-Luz Lopez-Rodrigues and all her colleagues from the Spanish Society of Medicinal Chemistry for their key role in organising this event. We already started exploring the possibilities for the third edition, which will take place in 2011, most probably in the Scandinavian Region.

Besides these key-events, which are organized or co-organised directly by EFMC, we sponsored numerous scientific events organised by our National Adhering Organisations. Among them, I particularly want to mention our educational events, the Medicinal Chemistry Schools. Besides the Summer School in Urbino (Italy), which is the only accredited school by now, EFMC supports also Medicinal Schools in Leiden (The Netherlands), Leysin (Switzerland), Nottingham (UK) and Vienna (Austria). This year, the Executive Committee also approved the application of the Summer School on Pharmaceutical Analysis (Italy), organised by Vincenza Andrisano. Welcome on board!

In June, on occasion of the 6th Joint Meeting on Medicinal Chemistry, organised in Budapest, the Council approved the proposal to join the Royal Chemical Society in launching a new journal, Medicinal Chemistry Communications (MedChemComm). Starting a new journal is not only a challenge, it is also a big responsibility and requires the commitment of all of us. The two editors in chief, Gregory Verdine from Harvard and Anthony Wood from Pfizer are in place and two out of three regional editors accepted the invitation. MedChemComm will focus on concise articles and reviews, and the submission site will go online very soon, so have a look and submit your article. It's a tough time schedule and we hope to have the first issue ready for distribution at the ISMC in Brussels.

In 2010, the most important event will be the 21st International Symposium on Medicinal Chemistry (EFMC-ISMC), organised by our two Belgian Member Societies in Brussels, Sep 5-9. The registration is already open, so please

do not miss to register to this most important Medicinal Chemistry event for this year. As for previous editions, the meeting will cover all major therapeutic areas, new technologies and hot topics. Special emphasis will be put on case studies and first time disclosures. On occasion of this event, also the three EFMC Awards will be conferred. These are 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. For the first time EFMC will also acknowledge a young medicinal chemist from Industry and one from Academia. The call for applications for the awards and the prizes is open till end of January, and I strongly encourage you to have a look on our web-page www.efmc.info for further information and to submit an application.

In November 2009 the second call of the Innovative Medicines Initiative has been published and applications are due on Feb 8. Further information as well as detailed reports on selected events mentioned above can be found in our newsletter MedChemWatch. I want to take the occasion to thank Gabriele Costantino and his team for their fantastic work. MedChemWatch develops extremely well and it is nice to see how the visibility and impact steadily increases.

Finally, I want to take this occasion to thank all members of the Executive Committee for the friendly and very constructive atmosphere we had during the whole year. I also wish to express my gratitude to the members of the Council, our committees and all colleagues who participated in the organization of our events. With the help of all of you we are looking forward to another productive and successful year for EFMC.

With my very best regards
Gerhard Ecker
President EFMC

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EFMC Premium Sponsors are CROs, Service Providers, Publishers that directly sponsor EFMC activities through major financial contributions. Their contribution helps the EFMC towards its main objective of developing a strong Medicinal Chemistry community in Europe that is well-equipped for the challenges of the future and enables the discovery of innovative new medicines for patients.



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EFMC offers any company the opportunity to become an official corporate member. Corporate membership will help EFMC with its objective of advancing the science of medicinal chemistry and can be achieved in several ways:

- By sponsoring an EFMC International Symposium with a minimum of €10 000
- By sponsoring an official EFMC Award
- By paying an annual fee of €2000 to EFMC

Companies interested to become a corporate member should contact Mark Bunnage at mark.bunnage@pfizer.com

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Medicinal Chemistry in Europe,
the Yearbook of the European Federation for Medicinal
Chemistry is published by:

LD Organisation sprl
Scientific Conference Producers
Rue Michel de Ghelderode 33/2
BE-1348 Louvain-la-Neuve, Belgium
Tel: +32 10 45 47 77 - Fax: +32 10 45 97 19
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The EC consists of seven members: the President, the President Elect or the Past President, the Secretary, the Treasurer and three additional members. All members of the EC, except the President and the Past President, are elected by secret ballot by the Council during a meeting of the Council. After a term of one year, the President Elect will automatically become President.

The members of the EC are not delegates of their respective countries. All details about the election process can be found in the statutes of the EFMC on the EFMC official website: www.efmc.info

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Activities

The current affairs of the Federation are handled by the EC. Among its members, the EC will assign the responsibilities of International Liaison, Communication and Planning.

Council

The Council consists of the members of the EC and one delegate of each Adhering Organisation. According to the statutes, the voting rights are allotted according to the following rules: members of the EC: 1 vote, countries with up to 99 members: 2 votes, countries with 100-199 members: 3 votes, countries with 200-399 members: 4 votes, countries with 400-599 members: 5 votes, countries with 600-899 members: 6 votes, countries with more than 899 members: 7 votes. As for countries with more than one Adhering Organisation, votes will be proportionally distributed among them, taking into account a resulting number will be rounded off to the closest digit.

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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 the 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. Moreover, it offers medicinal chemists an opportunity to present their work internationally by organising the biennial International Symposium on Medicinal Chemistry (EFMC-ISMC). These symposia, with an average attendance of 1,200 delegates, are highly international with a broad range of speakers and attendees representing well in excess of 40 countries.

The EFMC pursues its activities via the Executive Committee, the Council and 3 Committees devoted to Education and Training, Industry Liaison and Information & Communication. These Committees strengthen the links between Council and EC and help to define the mission, vision and goals of EFMC.

The EFMC has very strong links with the Medicinal Chemistry Division of the American Chemical Society. Through this collaboration the ACS convenes sessions for the biennial ISMC Symposia, and conversely the EFMC convenes sessions for ACS National meetings. In addition, the two societies regularly exchange observers at their committee meetings. Furthermore, the EFMC has a specific representative on the Editorial Advisory Board of the Journal of Medicinal Chemistry, thus demonstrating the quality of European science and its scientists. EFMC also has strong links with the European Federation for Pharmaceutical Sciences (EUFEPS). Besides

exchanging sessions at various scientific congresses, EFMC and EUFEPS joined forces in establishing a European Pharmaceutical Sciences Leadership Forum. EFMC also reaches out to former USSR and Eastern European scientists through its successful series of ASMC Symposia, organised with the support of ChemBridge Corporation, in Russia or in Ukraine. In addition, the EFMC also collaborates with the Asian Federation of Medicinal Chemistry by participating in meetings organised by the AFMC and vice versa, giving the EFMC a broad international footprint.

An important part of the EFMC activities is sponsorship of national scientific meetings and Medicinal Chemistry Schools. Supported by Bentham, it also awards bursaries for younger scientists to attend ISMC meetings. The EFMC also acknowledges the excellence of medicinal chemists' work, by conferring three major awards: the Nauta Award on Pharmacochimistry, the UCB-Ehrlich Award for Excellence in Medicinal Chemistry and the Prous Institute-Overton and Meyer Award for New Technologies in Drug Discovery, which are given every two years for outstanding achievements in the field of Medicinal Chemistry. From 2010 on, EFMC establishes two new prizes to acknowledge the scientific accomplishments of young medicinal chemists, both in industry and academia.

The EFMC homepage is now hot-wired to the web sites of many national organisations, thus facilitating the flow of information, and the e-newsletter MedChemWatch as well as the yearbook "Medicinal Chemistry in Europe" help to further develop cooperation between member organisations as well as their industrial partners and therefore advance medicinal chemistry in Europe, and by extension, around the globe.

Education and Training Committee

Current Committee Membership:

- Péter MÁTYUS – ETC Chair (EFMC Executive Committee Member, Hungary)
- Javier FERNANDEZ (EFMC Executive Committee Member, Spain)
- Danijel KIKELJ (EFMC Council Member, Slovenia)
- Peter MOHR (EFMC Council Member, Switzerland)
- Giuseppe RONSISVALLE (Università degli Studi di Catania, Italy)
- Alan STOBIE (Pfizer, United Kingdom)
- Henk TIMMERMAN (EFMC Council Member, The Netherlands)
- Anna TSANTILI-KAKOULIDOU (EFMC Council Member, Greece)

Committee Objective:

To ensure the training of the next generation of medicinal chemists within Europe at both the undergraduate and postgraduate levels, based on strong industry-academia cooperation, and to provide a platform to address future development training needs.

Committee Goals:

- Undertake a comprehensive analysis of the structure and profile of European teaching and education systems for medicinal chemistry
- Agree the core skills medicinal chemists should acquire during their Masters level and PhD level training
- Quantify existing undergraduate and postgraduate level training courses within Europe
- Identify best practice from this analysis and publish an overview and conclusions
- Summarise career destinations for Masters and PhD level medicinal chemists, and identify core skills gaps in each country from both the industrial and academic perspective
- Identify deficiencies in the current teaching and education of medicinal chemistry in Europe, and establish means of addressing these
- Summarise currently available software for e-learning of medicinal chemistry

- Continue to support the European School of Medicinal Chemistry (Urbino), accredited by EFMC, and the official EFMC sponsored schools; the Leiden/Amsterdam Center for Drug Research School on Medicinal Chemistry, the Swiss Course on Medicinal Chemistry, the Vienna Summer School, the Residential School: Medicinal Chemistry (Nottingham) and the Summer School on Pharmaceutical Analysis (Rimini)
- Facilitate the establishment of additional local residential Medicinal Chemistry Schools in other European countries
- Incorporate medicinal chemistry trends in future Medicinal Chemistry Schools
- Include sessions on the teaching and education of medicinal chemistry on a regular basis in EFMC-sponsored symposia
- Hold a satellite session at each ISMC on the future trends and direction of medicinal chemistry
- Raise the awareness and importance of appropriate medicinal chemistry training and education with other relevant learned societies e.g. IUPAC, EUFEPS

In order to achieve these challenging goals the Education Committee would welcome your knowledge, experience and ideas. If you wish to contribute towards our objectives, please contact Péter Mátyus at peter.matyus@szerves.sote.hu

Industry Liaison Committee

Current Committee Membership:

- **Mark BUNNAGE – ILC Chair** (EFMC Executive Committee Member, United Kingdom)
- **Javier FERNANDEZ** (EFMC Executive Committee Member, Spain)
- **David ALKER** (EFMC Council Member, United Kingdom)
- **Brigitte LESUR** (Institut de Recherches Servier, France)
- **Graeme ROBERTSON** (Siena Biotech, Italy)

Committee Objective:

To promote and improve liaison and cooperation between EFMC and Industry so that the EFMC can better achieve its over-arching objective to advance the science of medicinal chemistry. This includes increasing the visibility of EFMC activities within companies which employ medicinal chemists as well as those related industries for whom medicinal chemistry is an enabling science or for whom medicinal chemists represent a significant customer base.

- To encourage, recognise & support medicinal chemistry talent in industry (e.g. through EFMC prizes, industry sessions at EFMC meetings, etc)
- To support sharing of job offers and candidate CV through the EFMC website
- To establish a directory of European centres of specific expertise in drug research

Committee Goals:

- To act as a link between industry and academia for the exchange of ideas, information and knowledge on medicinal chemistry
- To understand and champion the views of industry within EFMC and, where appropriate, to promote these on a wider, European stage
- To provide a forum for industrial and academic medicinal chemists to discuss the evolution of medicinal chemistry in Europe

In order to achieve these challenging goals the ILC would welcome new committee members. If you are interested please contact Mark Bunnage at mark.bunnage@pfizer.com

Information & Communication Committee

Current Committee Membership:

- | | |
|------------------------------|--|
| • Koen AUGUSTYNS – ICC Chair | (EFMC Executive Committee Member, Belgium) |
| • Gabriele COSTANTINO | (Università degli Studi di Parma, Italy) |
| • Anders KARLÉN | (EFMC Council Member, Sweden) |
| • Jordi MESTRES | (Universitat Pompeu Fabra, Spain) |
| • László MOLNÁR | (Gedeon Richter, Hungary) |
| • David REES | (Astex Technology, United Kingdom) |
| • Yves ROLLAND | (EFMC Council Member, France) |

Committee Objective:

To improve and strengthen the communication to the EFMC member societies and individual Medicinal Chemists. The main goals are to increase the visibility of the EFMC and its activities via extensive use of internet-based technology and to establish an information platform for all issues related to Medicinal Chemistry in Europe. In addition, the ICC Committee will also support the other Committees in coordinating their activities and disseminating information.

- To explore possibilities for creating benefits for Corporate Members and individual Medicinal Chemists who are members of our National Adhering Organisations

In order to achieve these challenging goals the committee is open to suggestions and comments. Please send your ideas to Koen Augustyns at koen.augustyns@efmc.info

Committee Goals:

- To strengthen and improve communication with our National Adhering Organisations
- To support the National Adhering Organisations by ensuring that their information is communicated electronically in an efficient manner via EFMC channels
- To provide a Web-portal for Medicinal Chemistry activities in Europe and to broadly disseminate information on EFMC sponsored events

Editor

- Gabriele COSTANTINO (University of Parma, Italy)

Editorial Committee

- Erden BANOGLU (Gazi University, Turkey)
- Leonardo SCAPOZZA (Université de Genève, Switzerland)
- Wolfgang SIPPL (Martin-Luther-Universität Halle-Wittenberg, Germany)
- Kristian STROOMGARD (The Danish University of Pharmaceutical Sciences, Denmark)
- Mark LANSDELL (Pfizer, United Kingdom)

MedChemWatch will provide you with regular updates on the activity of our committees, give information on EFMC-approved schools and EFMC-sponsored meetings, and alert you on calls for medicinal chemistry related grants and funding opportunities. Furthermore, in each issue you will find a perspective article from a leading scientist and the presentation of a Medicinal Chemistry research group in Europe.

With MedChemWatch we intend to provide more than just one of those e-mails announcing the next meeting and promoting some activities. This should become a forum for exchange of ideas, thoughts and visions for the future of Medicinal Chemistry, accompanied by useful information on events, grants and news from our member societies.



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ASMC 2009

Report

3rd International Symposium on Advances in Synthetic and Medicinal Chemistry

Kiev, Ukraine, August 23 - 27, 2009

ASMC 09 in Kiev was organised by EFMC and ChemBridge Corporation, in the series of events which started with ASMC 04 in Moscow, followed by ASMC 07 in St. Petersburg. Prof. Erick Carreira (ETH Zürich, Switzerland) and Dr Scott Biller (Novartis Institutes for BioMedical Research, Cambridge, USA) were the Chairmen of this Symposium, where American and Western European chemists met Eastern European scientists in the areas of synthetic and medicinal chemistry.

The third edition of ASMC can be considered as a high point of the world's chemistry events of 2009, with 36 distinguished academic and industrial speakers, 10 oral communications and 81 poster presentations. ASMC 09 attracted about 300 participants, coming from 33 different countries, and 17% originating from former USSR countries. 36% of the attendees were from academia, 47% from industry.

The topics covered during the symposium included: New Synthetic Methodologies, Total Synthesis of Natural Products and Heterocyclic Chemistry, Diversity- and Target-Oriented Synthesis and Chemical Biology, Medicinal Chemistry and Drug Discovery & Development.

The outstanding scientific programme was completed by an attractive cultural programme. All participants have been invited to attend a guided bus tour of Kiev and had the opportunity to participate in the excursion to Lavra. Kiev, a lively and culturally rich city

on the banks of the Dnieper River, turned out to be a surprising destination and well worth the visit. In addition to this, Enamine, the main sponsor of the symposium, opened their doors and allowed interested participants to have a closer look at their laboratories. The warm welcome by the local participating companies helped making of ASMC 09 a successful event.

The programme also included a commercial exhibition and a half day Business Mini-Symposium.

The next ASMC will take place in 2011 in Moscow.



Frontiers in Medicinal Chemistry: Emerging Targets, Novel Candidates and Innovative Strategies

Barcelona, Spain, October 4-6, 2009

Last October the International Meeting "Emerging Targets, Novel Candidates and Innovative Strategies" took place in Barcelona (Spain). This event was the second in the series "Frontiers in Medicinal Chemistry" initiated in Siena (Italy) in 2007. On this occasion and under the auspices of the European Federation of Medicinal Chemistry (EFMC) and the Spanish Society of Medicinal Chemistry (SEQT), the meeting has brought medicinal chemists and related scientists together in order to share exciting new results and first-time disclosures in the different areas of drug discovery and development.

Toward this aim, twenty-three internationally recognized invited speakers presented the current trends on emerging targets, novel drug candidates and new strategies and technologies. Additionally, two poster sessions showed the latest results on a wide range of medicinal chemistry topics.

Inaugurated by the presidents of the EFMC, Gerhard Ecker, and SEQT, María Luz López-Rodríguez, the Symposium was opened with the lectures of Prof. Luis Serrano (Centre for Genomic Regulation, Spain) and Prof. Leonardo Pardo (Universitat Autònoma de Barcelona, Spain). During the following days, professors, lecturers, students and representatives of the pharma industry attended a busy programme organised in twenty half hour lectures and two poster sessions, which covered all key aspects of medicinal chemistry including sessions on CNS, pain, cancer, infectious diseases, inflammation, metabolic disease and chemical biology.

The meeting concluded with the outstanding presentation delivered by Prof. Gregory L. Verdine (Harvard University, USA) and the EFMC and SEQT awards to posters presented by young researchers.

Besides the scientific aspects of the programme, Barcelona as the host city had many cultural highlights and tourist attractions and all of the participants enjoyed the fantastic venue of the meeting as well as the weather during those days.

This symposium fulfilled its primary objective, which was to provide a dynamic environment to foster interaction and discussion and to contribute to strengthen ties between scientists. Of the total of 298 participants, slightly more than one third belonged to the pharmaceutical industry of a wide variety of countries.

"Frontiers in Medicinal Chemistry" was made possible by the generous financial support of our institutional and industrial sponsors and the assistance of our collaborators. Also, the organising and scientific committee would like to acknowledge the speakers and participants for sharing their science and, more importantly, for their key contribution to the outstanding scientific level of the event.





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- The Nauta Award for Pharmacocchemistry
- 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 Young Medicinal Chemist in Industry
- Prize for Young Medicinal Chemist in Academia

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COVALENT INHIBITORS IN DRUG DISCOVERY

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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)

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G-PROTEIN COUPLED γ TM RECEPTORS - NEW INSIGHTS INTO THEIR STRUCTURE AND LIGAND RECOGNITION

Hans Bräuner-Osborne
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EFMC 2010 AWARDS

Call for nominations

DEADLINE: JANUARY 31, 2010

Nominations for these Awards consist of a nomination letter, a brief CV, including a list of selected publications and two supporting letters. The nominations should be submitted to the Chairman of the Juries, Professor Gerhard Ecker, President of EFMC, Department of Medicinal Chemistry, University of Vienna, Althanstrasse 14, A-1090 Wien, Austria. fax: +43 1 4277 9551 e-mail: awards@efmc.info



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Applications 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

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Nominations should be submitted by the candidate's supervisor and should consist of:

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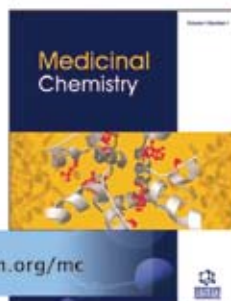
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Calendar of Events

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Young Research Fellow Meeting

**February 5, 2010
Paris, France**

www.sct-asso.fr

Contact Person: Luc Demange
Tel: +33 153739685
Email: luc.demange@univ-paris5.fr

Organised by:
Société de Chimie Thérapeutique (France)

Frontiers in Medicinal Chemistry

**March 14-17, 2010
Münster, Germany**

www.gdch.de/medchem2010

Contact Person: Prof. Dr Bernhard Wunsch
Tel: +49 251 83 33311
Fax: +49 251 83 32144
Email: wwunsch@uni-muenster.de

Organised by:
Division of Medicinal Chemistry of the German
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German Pharmaceutical Society, Section of
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Spring Symposium : Crossing Decades and Borders in Medicinal Chemistry

**March 19, 2010 Eindhoven,
The Netherlands**

Contact Person: Jac Wijkmans
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Email: jac.wijkmans@spcorp.com

Organised by:
Section Medicinal Chemistry,
Royal Netherlands Chemical Society (KNCV)

Joint Meeting SCT - SFC - Académie Nationale de Pharmacie (ANP)

**March 23, 2010
Paris, France**

www.sct-asso.fr

Contact Person: Robert Dodd
Email: robert.dodd@icsn.cnrs-gif.fr

Organised by:
Société de Chimie Thérapeutique (France),
French Society of Chemistry, French National
Academy of Pharmacy

**2nd Short Course on Medicinal Chemistry -
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Henk Timmerman, VU Amsterdam, NL

www.efmcshortcourses.org
Contact: administration@efmc.info

Organised by:
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www.efmc.info

14th Hellenic Symposium on Medicinal Chemistry

**April 23-25, 2010
Thessaloniki, Greece**

www.helmedchem2010.gr

Contact Person:
Vassilis Demopoulos
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Email: vdem@pharm.auth.gr

Organised by:
Hellenic Society of Medicinal Chemistry (Greece)
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Chemistry of the Association of Greek Chemists
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**28th Camerino-Cyprus-Noordwijkerhout
Symposium
Trekking Through Receptor Chemistry**

**May 16-20, 2010
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www.unicam.it/farmacia/symposium/index.html

Contact:
Dipartimento di Scienze Chimiche
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Email: secretariat.camerino@unicam.it

Organised by:
Medicinal chemistry Division
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Minisymposium on «Channels and Transporters»

**May 27, 2010
Institute of Organic Chemistry, University of Basel**

Contact Person:
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Fax: +41 61 688 6459
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Organised by:
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Swiss Chemical Society (SCS) (Switzerland)

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(SSPA 2010)**

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www.scpaweb.org

Contact Person:
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**RICT2010 - 46th International Conference
on Medicinal Chemistry - 46^{èmes} Rencontres
Internationales de Chimie Thérapeutique**

**June 30 - July 2, 2010
Reims, France**

www.medchem.fr

Contact Person:
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Email: janos.sapi@univ-reims.fr

Organised by:
Société de Chimie Thérapeutique (France)

European School of Medicinal Chemistry (ESMEC)

**July 4-9, 2010
Urbino, Italy**

www.esmec.eu

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www.ismc2010.org/

Contact Person:
Dr Edmond Differding (UCB S.A.)

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Chemistry Division (Belgium)

**XXth National Meeting
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**September 12-16, 2010
Abano Terme (Padova), Italy**
www.nmmc2010.sistemacongressi.com

Contact Person:
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Email: francesco.dallacqua@unipd.it

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Chemical Society (Società Chimica Italiana) (Italy)

**Medicinal Chemistry Section at Fall Meeting
of the Swiss Chemical Society**

**September 16, 2010
ETH Zürich, Switzerland**

Contact Person:
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**18th European Symposium on Quantitative
Structure – Activity Relationships**

**September 19-24, 2010
Rhodes, Greece**

www.euroqsar2010.gr

Contact Person:
Prof. Anna Tsantili - Kakoulidou
Tel: + 30 210 7274530 - Fax: +30 210 7274 747
Email: tsantili@pharm.uoa.gr

Organised by:
Hellenic Society of Medicinal Chemistry (Greece)
and International Cheminformatics
and QSAR Society

**3rd RSC-SCI Symposium on GPCRs in
Medicinal Chemistry**

**September 20-22, 2010
Schering-Plough, Oss, The Netherlands**

www.rsc.org/bmcs

Contact Person:
Dr Caroline Low
Email: c.low@imperial.ac.uk

Organised by:
The Biological and Medicinal Chemistry Sector
(BMCS) of the Royal Society of Chemistry (RSC)
(United Kingdom), SCI-FCG

3rd Polish Meeting on Medicinal Chemistry

**September 20-22, 2010
Lublin, Poland**

www.ptchm.pl

Contact Person:
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Fax: + 48-81-535 73 55
Email: ptchm@ptchm.pl / darek.matosiuk@am.lublin.pl

Organised by:
Polish Society of Medicinal Chemistry (Poland)

**5th IMMPC (International Meeting on
Medicinal and Pharmaceutical Chemistry)**

October 2010 Istanbul, Turkey

Contact Person:
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Fax: + 903051872/120
Email: epalaska@hacettepe.edu.tr

Organised by:
Turkish Association of Medicinal and Pharmaceuti-
cal Chemistry (Turkey)

FIGON Dutch Medicine Days

**October 4-6, 2010
Lunteren, The Netherlands**

www.figon.nl

Organised by:
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19th LACDR School on Medicinal Chemistry

**October 19-22, 2010
Noordwijkerhout, The Netherlands**

www.lacdr.nl

Organised by:
Section Medicinal Chemistry, Royal Netherlands
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9th Swiss Course on Medicinal Chemistry

**October 10-15, 2010
Leysin, Switzerland**

www.swiss-chem-soc.ch/smc/leysin/leysin.html

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Organised by:
Division for Medicinal Chemistry (DMC), Swiss
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IXth Jornadas de la SEQT

**November 2010
Baeza-Jaén, Spain**

www.seqt.org

Contact Person:
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Email: jmcampos@ugr.es

Organised by:
SEQT/Granada University
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RSC-SCI Flow Chemistry Symposium

**November 3-4, 2010
GSK, Stevenage**

www.rsc.org/bmcs

Contact Person: Dr Jason Tierney
Email: jason.tierney@glpg.com

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The Biological and Medicinal Chemistry Sector
(BMCS) of the Royal Society of Chemistry (RSC)
(United Kingdom) and BMCS/SCI-FCG

**SCT Annual Workshop
in Medicinal Chemistry**

**December 2010
Paris, France**

www.sct-asso.fr

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- Templates for DOS
- Elements for SFBDD
- Privileged structures
- Building blocks
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Achievements and Challenges for Similarity Searching

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The term ‘virtual screening’ has emerged in the 1990s describing a rather loosely defined set of computational approaches to predicting novel bioactive compounds. Ever since, methods for automated ligand-receptor docking and techniques for molecular similarity searching have emerged as workhorses for computational and medicinal chemists alike to assist in the task of compound selection for activity screening and hit-to-lead optimization (1-6). There is no longer doubt that a smart application and combination of virtual screening tools can actually help find novel chemotypes with a desired pharmacological activity profile (7-9).

While in the early years mere hit identification, library shaping, and rapid database searching was pursued, more advanced tasks are being aimed at today, such as scaffold- or lead-hopping (10, 11), multi-dimensional (multi-objective) optimization of lead structure properties

(12), repurposing of known drugs (13, 14), prediction of activity profiles rather than individual targets (15-17), just to name a few. Most importantly, as a main lesson from many virtual screening studies, it has been realized that ‘similarity’ between two molecules is a context- and target-dependent property, and cannot be expressed by a single universally applicable compound representation or description.

As a general guideline for rapid first-pass similarity searching, it is advisable to represent molecules by shape and pharmacophoric features (Fig. 1). Although this concept has been known for many years, it has been re-discovered for practical virtual screening that these two features capture essential aspects of receptor-drug interactions (18, 19). Ideally, such models implicitly code pharmacologically important molecular properties like lipophilicity. While atomistic and substructure-based molecular descriptors

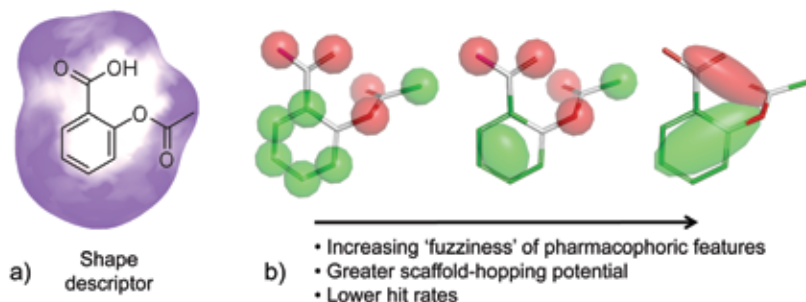


Figure 1. Representation of acetyl salicylic acid by shape (a) and various degrees of 'fuzzy' pharmacophoric points (b). Here, green ellipsoids represent lipophilic centers and red ellipsoids indicate polar, potentially hydrogen-bonding sites. Depending on the degree of abstraction, atomistic models and coarse-grained pharmacophoric models can be obtained. It is important to realize that hit rates in real screening usually decrease with increasing 'fuzziness' of the molecular representation that was used for screening compound selection by similarity searching.

(e.g., 'fingerprints' like MACCS keys (20), Ghose-Crippen fragment keys (21)) are preferred for compound database searching aiming at the rapid retrieval of derivatives of a particular underlying chemotype, shape and pharmacophore descriptors facilitate the identification of bioisosters and scaffold-hops (22-24). It is safe to say that with an increasing abstraction from atom-and-bond (molecular graph-based) models fewer similar but more diverse chemotypes are retrieved from a compound database, which immediately mirrors in reduced hit rates. It is mandatory to realize and accept this dependency, as there are sometimes unrealistically high expectations of hit rates and abundant novel scaffolds among the hits. A weak hit compound featuring a novel scaffold can be a valuable starting point for additional rounds of virtual screening that eventually lead to potent lead structures.

To illustrate the potential of concerted virtual screening, modeling and optimization, an example is presented in Fig. 2.

Starting from a known cannabinoid-1 receptor (CB1R) ligand, researchers at Roche employed pharmacophore-based de novo design for scaffold-hopping and first hit identification (25), which was followed by further refinement by pharmacophore compliance, chemical tractability, and drug-likeness considerations, and eventually resulted in a series of benzodioxoles as potent novel CB1R inverse agonists. This strategy of extensive multidimensional optimization involved tight interaction between virtual and real screening and was rewarded by the identification of promising lead compounds with significant in vivo activity (26).

Another hallmark example of broad virtual screening and similarity searching in tight combination with real screening has recently been given by Roth and coworkers who found several new targets for marketed drugs and conclude that "*The chemical similarity approach is systematic and comprehensive, and may suggest side-effects and new indications for many drugs.*" (14)



Figure 2. Example of a strategy for multidimensional optimization by iteratively applied virtual screening methods. Starting from the known cannabinoid-1 receptor (CB1R) effector **1** ($K_i = 0.11 \mu\text{M}$) (**51**) as a reference compound, fragment-based *de novo* design with the software TOPAS (**52**) led to weakly active hits **2** in small combinatorial libraries that were derived from design. Using these hit compounds as queries for pharmacophore-based similarity assessment and subsequent medicinal chemical optimization finally resulted in lead compound **3** ($K_i = 0.03 \mu\text{M}$), a potent CB1R agonist featuring a novel scaffold compared to the original reference **1**.

Guidelines for fast and successful similarity searching

There are some basic guidelines for first-pass virtual screening by *similarity searching* that may be deduced from various recent research reports. These tips should be understood as empirical findings (supported by personal experience and preferences) rather than analytically obtained rules:

- Use all potent reference compounds as queries. This will increase the chance of finding potent hits (27).
- Describe molecules by their topology or shape plus pharmacophoric features to capture two complementary molecular features that are generally relevant for ligand-receptor interaction (23, 24).
- Whenever possible, describe molecules by few features (28). This will help avoid artifacts resulting from high-dimensional compound descriptions (the “curse of dimensionality”) (29).
- For each of the molecular representations perform individual similarity searches in large compound collections (30). This will help increase the number of different chemotypes among the top-scoring compounds.
- Compute pair-wise molecular similarity by two complementary techniques: a *metric* (e.g., Manhattan distance, Euclidian distance) and a *similarity index* (e.g., Tanimoto-index) (29). This can help avoid artificial bias towards certain chemotypes.
- Combine individual ranked compound lists, e.g. by ‘group fusion’ (31, 32).
- Trust the results and consider the top-scoring compounds for biochemical testing, irrespective of your own or your colleagues’ opinion.

- Look at the top-scoring compounds and select additional screening candidates manually.

In any case, at least two subsequent rounds of virtual and real screening should be performed before an assessment of the overall outcome of the screening campaign should be made. Numerous studies have shown that initial weak hits can be optimized to potent ligands in subsequent select-and test cycles. It is always a good idea not to blow all screening capacity in one shot but to learn in iterative steps. This can be done, for example, by using initially poor hits as queries for a second or third virtual screening triage (33).

Notably, a description of ‘two-dimensional’ molecular structure (in particular descriptors of molecular topology) has repeatedly led to surprisingly good results. One reason might be that three-dimensional representations by shape and pharmacophores as well as molecular docking methods have to explicitly cope with conformer generation and flexibility, while some of the available topological descriptors have the ability to implicitly capture relevant aspects of conformational preferences and restrictions (34, 35). This does by no means render three-dimensional approaches like docking useless but pinpoints to a general issue of virtual screening protocols. Recently, Bajorath and coworkers successfully transferred information about relevant receptor-ligand interaction sites from three-dimensional binding complexes to two-dimensional fingerprints, which resulted in improved hit rates (36).

What's next?

Ignoring various technological aspects, publication policies, the ‘human factor’ and obvious project-specific considerations, it is fair to say that a main achievement of virtual screening as a whole has been to provide methods that help eliminate the bulk of inactive compounds, rather than actually predict actives (37). While this statement is certainly simplifying (and grossly inadequate for individual studies and techniques) it pinpoints to one of the major limitations we are currently facing, namely the *accurate and rapid* quantitative computation of binding free energies (respectively pK_d , pIC_{50}) for arbitrary ligand-receptor complexes (38). This poses a problem not only for three-dimensional receptor-ligand and protein-protein docking (scoring problem (39, 40)) but also for advanced QSAR techniques and machine learning approaches. While there are elegant and analytically exact algorithmic solutions for compound placing in a binding site and mathematical model finding and optimization, we still lack sufficiently accurate approximations of basic physical and chemical phenomena of receptor-ligand binding or fail to model them with sufficient accuracy within a reasonable time. These include in particular

- entropic contributions to ligand binding
- dynamic behavior of both ligands and macromolecular targets
- role of solvent (water, ions) in complex formation and stability

- dynamic conformational ensembles of ligands and ligand-receptor complexes.

Explicit consideration of the flexibility of ligands and receptors in docking and pharmacophore modeling has already led to some progress. For example, ligand-based virtual screening by *pseudo*-receptor models (41) was combined with molecular dynamics simulations to obtain ligand binding sites in comparative protein models ('homology' models) of the histamine H4 receptor, a G-protein coupled receptor (42). Comparative protein models have also gained attractiveness for ligand docking and scoring during the last year due to developments in consensus scoring and flexibility considerations (43). DOCK Blaster is an expert system for unsupervised high-throughput ligand docking with multiple targets that reassesses the correctness of ligand binding poses in three-dimensional protein models (44). Another innovative concept was realized in the HYDE scoring function, namely the use of $\log P$ -derived atomic increments for the computation of free dehydration and hydrogen bonding energies, which resulted in improved accuracy and in particular fewer false-positives (45).

While these approaches focus on complex scoring and molecular flexibility, other seemingly trivial problems remain largely unsolved until now, for example the accurate prediction of tautomerization equilibria (46) or computation of pK_a values (47, 48).

Developments in computer hardware have always led to an improvement of

modeling capabilities. We are currently witnessing an exciting development of specialized graphics processor chips and parallel computing technology as potential workhorses for molecular dynamics and other computationally very demanding calculations (49, 50). No doubt this will enable long time (beyond 100 ns) dynamics simulations of macromolecular targets on a routine basis, which can help understand allosteric effects, flexible fit phenomena of druglike ligands and effector molecules (51). As a consequence, dynamic molecular features (in contrast to 'static' properties like molecular mass, $\log P$, and other time-invariant molecular properties) that cannot be accurately modeled today, will be within our grasp and improve the accuracy of future predictions of novel bioactive compounds.

Acknowledgements

I am very grateful to Herbert Köppen, Tim Clark, Nikolaus Heinrich, and Karl-Heinz Baringhaus for stimulating discussion of the myths and facts of virtual screening.

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Website	http://www.kvcv.be
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Activities	Annual meetings, interdisciplinary symposia, scientific publications, award. Frontiers in Medicinal Chemistry (March 14-17, 2010), Münster, Germany
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NAO Secretariat

The Medicinal Chemistry Section of the Israel Chemical Society



Mission	To organise and to foster the interaction between medicinal chemists in academia, industry and drug dispensing institutions, in an independent association devoted to education, research and development of Medicinal Chemistry through meetings and workshops, and to represent the Association at the national level, at the EPMC, and at related international levels. IAMC is open for membership to molecular biologists, pharmacologists and pharmacists.
Founded	1991, 2004 - united with the Israel Association for Medicinal Chemistry
Members	200
Member profile	Trade and Industry: 35% Research Institute and University: 60% Other: 5%
Postal address	Department of Medicinal Chemistry and Natural Products School of Pharmacy – Faculty of Medicine Hebrew University of Jerusalem PO Box 12065 91120 Jerusalem Israel
Telephone	+972-2675-75-73, cell: +972-52-4282677
Fax	+972-2675-70-76
E-mail	avid@ekmd.huji.ac.il
Website	http://www.weizmann.ac.il/conferences/medchem/
Activities	The Association holds symposia and annual scientific meetings. Promotion of one-day symposia on new vistas in drug research and a workshop on progress in instrumental drug analysis, and representation of the Association at the EPMC and related international bodies.
President	Prof. Dr Abraham DOMB J. (Hebrew University of Jerusalem)
EFMC-Delegate	Dr Jeffrey STERLING (TEVA Pharmaceutical Ind.)
NAO Secretariat	ICS (Medicinal Chemistry Section)



Division of Medicinal Chemistry of the Italian Chemical Society (Società Chimica Italiana)

To improve Medicinal Chemistry in academia and industry by promoting contacts and collaboration between researchers working in this and related fields with the aim to propose and develop projects to advance Medicinal Chemistry; to organise national and international meetings, interdisciplinary symposia and advanced schools to spread knowledge in drug development; to distribute awards and grants that encourage junior scientists to pursue research in Medicinal Chemistry; to cooperate with similar associations in the country and abroad.

1979

600

Trade and Industry: 13%

Research Institute: 5,5%

University: 81%

Other: 0,5%

Divisione di Chimica Farmaceutica
University of Genova-Dipartimento di Scienze Farmaceutiche
Viale Benedetto XV, 3 - 16132 Genova, Italy

+ 39-010-353-8350

+ 39-010-353-8358

mosti@unige.it<http://dcf.frm.uniroma1.it/cgi-bin/home.pl>

Summer School on Pharmaceutical Analysis (SSPA 2010)

(June 14-16, 2010), Rimini, Italy

European School of Medicinal Chemistry (ESMEC)

(July 4-9, 2010), Urbino, Italy

XXth National Meeting on Medicinal Chemistry

(September 12-16, 2010), Abano Terme (Padova), Italy

Prof. Dr Luisa MOSTI
(University of Genova)

Prof. Dr Antonello MAI
(University of Rome La Sapienza)

Prof. Dr Carlo FRANCHINI
(University of Bari)

Prof. Dr Luisa MOSTI
(University of Genova)

Mission

Founded
Members
Member profile

Postal address

Telephone
Fax

E-mail
Website

Activities

President

Secretary

Treasurer

EFMC-Delegate

Founded	1992
Members	12
Member profile	Research Institute and University: 83% Other: 17%
Postal address	Latvian University Institute of Microbiology and Biotechnology 4-402 Kronvalda Boulevard LV-1586 Riga Latvia
Telephone	+371 7034890
Fax	+371 7323065
E-mail	vina@lanet.lv
Activities	Promotion of medicinal chemistry
President	Dr Ilmara VINA (Latvian University)
EFMC-Delegate	Prof. Dr Gunars DUBURS (Latvian Institute of Organic Synthesis)



Section of Pharmacochimistry, Royal Netherlands Chemical Society (KNCV)

To promote scientific research and education in the area of pharmacochimistry. To bring together scientists in the field and to offer them a platform for discussion and exchange of ideas. To identify talent in the field. To organise meetings in the field.

28th August 1970
350 (including student members)

Trade & Industry: 20%
Research Institute: 10%
University: 40%
Other: 30%

Dr J.C.H.M. Wijkmans
MSD
Department of Medicinal Chemistry, Room RK 3111
P.O. Box 20 - 5340 BH Oss
The Netherlands

+31-412-665464
+31-412-662546

jac.wijkmans@spcorp.com
www.kncv.nl

Organisation of one annual scientific meeting (1 day).
Co-organisation of Dutch Medicine Days (FIGON) (2 days).
Co-organisation of annual NWO platform meeting (2 days).
Co-organisation of sessions at KNCV Winter/Summer Congress.
Participation in KNCV, NWO, FIGON and EFMC platforms.
Dutch Medicinal Chemistry Award every 2 years for the best Dutch
Ph.D. thesis in the field.

Spring Symposium: Crossing Decades and Borders in Medicinal Chemistry

joint meeting with Société Royale de Chimie, Medicinal Chemistry
Division (SRC) and Medicinal and Bioorganic Chemistry Division of
Royal Flemish Chemical Society (KVCV)
(March 19, 2010), Eindhoven, The Netherlands

FIGON Dutch Medicine Days

(October 4-6, 2010), Lunteren, The Netherlands

19th LACDR School on Medicinal Chemistry

(October 19-22, 2010), Noordwijkerhout, The Netherlands

Prof. Dr A.P. IJZERMAN (Medicinal Chemistry / LACDR)
Dr J.C.H.M. WIJLMANS (MSD)

Dr H.K.A.C. COOLEN (Solvay Pharmaceuticals BV)

Prof. Dr Henk TIMMERMAN (Vrije Universiteit Amsterdam / LACDR)

Mission

Founded Members

Member profile

Postal address

Telephone Fax

E-mail Website

Activities

President
Secretary
Treasurer
EFMC-Delegate

Polish Society of Medicinal Chemistry



Mission	Basis for mutual contacts and integration for scientists who represent different profile of their activity in the following areas of medicinal chemistry: organic and bioorganic synthesis, analytical chemistry, computational chemistry, biochemistry, molecular biology, biotechnology, pharmacy and medicine.
Founded	2006
Members	50
Postal address	Jagiellonian University Medical College, Pharmacy Faculty Medyczna 9 30-688 Kraków Poland
Telephone	+48 12 620 55 81; +48 12 620 55 80
Fax	+48 12 620 55 96
E-mail	ptchm@ptchm.pl
Website	www.ptchm.pl
Activities	<ul style="list-style-type: none"> - Organisation of meetings where various theoretical and practical topics of drug research and development are discussed. - Participation in organisation of national and international conferences on medicinal chemistry. - Propagation of news and information on medicinal chemistry activity in the scientific society interested in medicinal chemistry. <p>Executive Committee Prof. Dr Andrzej BOJARSKI Prof. Dr Janina KAROLAK-WOJCIECHOWSKA Prof. Dr Katarzyna KIEC-KONONOWICZ Prof. Dr Dariusz MATOSIUK Dr Marek ZYLEWSKI</p> <p>3rd Polish Meeting on Medicinal Chemistry (September 20-22, 2010 Lublin, Poland)</p> <p>Prof. Dr Katarzyna KIEC-KONONOWICZ (Jagiellonian University)</p>
EFMC-Delegate	



Group of Medicinal Chemistry of the Portuguese Chemical Society

To diffuse the knowledge of Medicinal Chemistry.
To foster interdisciplinary bridges between Chemistry,
Biology, Medicine and Pharmacy.
To encourage research among young students.
To promote the interaction between medicinal chemists in
academia and professionals in industry.

2007

62

Sociedade Portuguesa de Química
Av. da República, 37-40
1050-187 Lisboa
Portugal

+351 21 793 4637

+351 21 795 2349

sede@spq.ptwww.spq.pt

Assisting and promoting regular courses in Medicinal Chemistry
targeted for (undergraduated and postgraduated) students.
Organisation of short meetings and seminars on recent advances
in the area of Medicinal Chemistry.

A National Meeting in Medicinal Chemistry is planned biennially.

Prof. Dr M. Luisa SÁ E MELO
(University of Coimbra)

Prof. Dr Rui MOREIRA
(University of Lisbon)

PCS
(Group of Medicinal Chemistry)

Mission

Founded Members

Postal address

Telephone Fax

E-mail Website

Activities

President

EFMC-Delegate

NAO Secretariat

The D.I. Mendeleev Russian Chemical Society

Medicinal Chemistry Section



Mission	Education in medicinal chemistry. Organisation of regular scientific seminars.
Founded	2000
Members	150
Member profile	Research Institute: 67% University: 26% Other: 7%
Postal address	RU-119899 Moscow Russia
Telephone	+ 7 095 939 1620
Fax	+ 7 095 939 0290
E-mail	zefirov@org.chem.msu.ru
Activities	Organising regular and specific seminars in medicinal chemistry. Assisting in the organisation of regular courses for undergraduate students of Moscow State University in medicinal chemistry. Providing interaction between Russian academician research in the field of medicinal chemistry and industrial institutions.
President	Prof. Dr Nikolay S. ZEFIROV (Moscow State University)
EFMC-Delegate	Prof. Dr Nikolay S. ZEFIROV (Moscow State University)



Serbian Chemical Society, Division of Medicinal Chemistry

To establish communication and co-operation between academia and industry, promote scientific research and education in the area of medicinal chemistry and encourage research among young students through meetings, seminars and workshops.

Industry 6%
Research Institute and University 86%
Others 4%

Karnegijeva 4
11120 Belgrade
Serbia

+381-11-3370-467
+381-11-3370-467

SHDOoffice@tmf.bg.ac.yu
www.shd.org.rs

Promotion of medicinal chemistry by academy-industry interaction, co-operations with other organisations and support of the education in medicinal chemistry.

Prof. Dr Miroslav J. GASIC
(Serbian Academy of Sciences and Arts)

Prof. Dr Dragana MILIC
(Faculty of Chemistry University of Belgrade)

Prof. Dr Miroslav J. GASIC
(Serbian Academy of Sciences and Arts)

Mission

Member profile

Postal address

Telephone Fax

E-mail Website

Activities

President

Secretary

EFMC-Delegate

Section for Medicinal Chemistry of the Slovenian Pharmaceutical Society



Mission	The mission of the Section for Medicinal Chemistry of the Slovenian society is the advancement and promotion of medicinal chemistry in Slovenia and Europe. It will pursue its mission by organising scientific meetings, schools and working-group in order to encourage discussions and exchange of ideas in the field of medicinal chemistry. This section will cooperate with similar associations in the country and abroad.
Founded	23 February 2004
Members	28
Member profile	Trade and Industry: 20 % Research Institute: 15 % University: 60 % Others: 5 %
Postal address	University of Ljubljana Faculty of Pharmacy Aškerceva 7 1000 Ljubljana Slovenia
Telephone	+386 1 4769561
Fax	+386 1 4258031
E-mail	danijel.kikelj@ffa.uni-lj.si
Website	www.sfd.si
President	Dr Lucija PETERLIN MAŠIČ (University of Ljubljana)
EFMC-Delegate	Prof. Dr Danijel KIKELJ (University of Ljubljana)



Sociedad Española de Química Terapéutica

To assist in the development and improvement of research and training in the different areas of Medicinal Chemistry throughout Spain.

1977

390

Trade & Industry: 25%
Research Institute: 30%
University: 35%
Other: 10%

Juan de la Cierva,3
28006 Madrid
Spain

+34 91 56 22 900

+34 91 56 44 853

seqt@iqm.csic.es
www.seqt.org

Supporting the participation of young researchers at meetings and other educational events. Organising symposia on topics related with research and education towards the discovery of new drugs.

Sponsoring the Spanish Society of Medicinal Chemistry Award.

Administering six Awards addressed to young scientists to acknowledge outstanding research in the field of Medicinal Chemistry.

IX Jornadas de la SEQT

(November 2010), Baeza-Jaén, Spain

Prof. Dr María L. LÓPEZ-RODRÍGUEZ
(Universidad Complutense de Madrid)

Dr Ana Rosa SAN FÉLIX GARCÍA
(IQM-CSIC)

Dr Sonsoles VELÁZQUEZ DÍAZ
(IQM-CSIC)

Prof. Dr María L. LÓPEZ-RODRIGUEZ
(Universidad Complutense de Madrid)

SEQT

(Sociedad Española de Química Terapéutica)

Mission

Founded Members

Member profile

Postal address

Telephone Fax

E-mail Website

Activities

President

Secretary

Treasurer

EFMC-Delegate

NAO Secretariat

The Swedish Academy of Pharmaceutical Sciences

Section for Medicinal Chemistry



Mission	To strengthen the Medicinal Chemistry Discipline through the arrangement of conferences, seminars and other educational initiatives.
Founded	1972
Members	276
Member profile	Trade & Industry: 70% Research Institute: 1% University: 19% Other: 10%
Postal address	Wallingatan 26A SE Stockholm Sweden
Telephone	+46 8 723 50 00
Fax	+46 8 20 55 11
E-mail	Agneta.Larhed@lakemedelsakademin.se
Website	www.swepharm.se
Activities	Symposia, seminars, courses.
President	Prof. Dr Anders KARLÉN (Uppsala University)
Secretary/ Treasurer	Anna-Lena GUSTAVSSON (Karolinska Institutet)
Secretary	Dr Agneta LARHED (Swedish Academy of Pharmaceutical Sciences)
EFMC-Delegate	Prof. Dr Anders KARLÉN (Uppsala University)



SCS
Division of
Medicinal Chemistry

Division for Medicinal Chemistry (DMC), Swiss Chemical Society (SCS)

The DMC provides a forum for scientists interested in medicinal chemistry and related fields by organising symposia, seminars, presentations and courses.

1990
580

Trade & Industry: 75%
University: 15 %
Other: 10%

Schwarztorstrasse 9
3007 Bern
Switzerland

+41 31 310 40 90
+41 31 310 40 29

info@scg.ch
www.scg.ch

Minisymposium on «Channels and Transporters»

(May 27, 2010), Institute of Organic Chemistry, University of Basel,
Switzerland

Medicinal Chemistry Section at Fall Meeting of the Swiss Chemical Society

(September 16, 2010), ETH Zürich, Switzerland

9th Swiss Course on Medicinal Chemistry

(October 10-15, 2010), Leysin, Switzerland

Dr Hans Peter MAERKI
(F. Hoffmann-La Roche)

Dr Peter MOHR
(F. Hoffmann-La Roche)

SCS
(Division for Medicinal Chemistry (DMC))

Mission

Founded Members

Member profile

Postal address

Telephone Fax

E-mail Website

Activities

President

EFMC-Delegate

NAO Secretariat

Turkish Association of Medicinal and Pharmaceutical Chemistry



Mission	Establish communication and cooperation between the members. Establish policies in medicinal chemistry teaching and research in the country. Organise scientific meetings and conferences, get in touch with international related bodies.
Founded	1994
Members	170
Member profile	Academics: 100%
Postal address	Department of Pharmaceutical Chemistry Faculty of Pharmacy - Gazi University 06330 Ankara Turkey
Telephone	+90 312 222 72 25
Fax	+90 312 223 50 18
E-mail	mfsahin@gazi.edu.tr
Website	www.medchem.org
Activities	5th IMMPC (International Meeting on Medicinal and Pharmaceutical Chemistry) (October 2010), Istanbul, Turkey
President	Prof. Dr M. Fethi SAHIN (Gazi University)
EFMC-Delegate	Prof. Dr M. Fethi SAHIN (Gazi University)



The Biological and Medicinal Chemistry Sector (BMCS) of the Royal Society of Chemistry (RSC)

The BMCS aims to further the interests of all members of the RSC, both industrial and academic, involved in the pursuit and understanding of biologically active molecules. It also acts to promote public awareness of the crucial role played by chemistry in the modern industrial environment.

1995 (Formerly Fine Chemicals & Medicinals Group)
897 in total; 600 of whom are medicinal chemists
Predominantly industry

Royal Society of Chemistry - Burlington House - Piccadilly
W1J 0BA London, United Kingdom
+44 207 437 8656
+44 207 437 8883

www.rsc.org/Membership/Networking/InterestGroups/BMCS

Mission

Founded
Members
Member profile

Postal address

Telephone
Fax
Website
Activities

The Biological and Medicinal Chemistry Sector (BMCS) is a Sector of the Industry & Technology Forum of the Royal Society of Chemistry (RSC) in the UK. The annually elected committee is primarily responsible for the organisation of scientific meetings and symposia, supporting educational activities in the UK, and advising the Society on policies that directly affect the BMCS. Specifically, the BMCS aims to further the interests of all members of the RSC, both industrial and academic, involved in the pursuit and understanding of biologically active molecules. The predominant areas thus include pharmaceuticals, agrochemicals, flavours and fragrances. It also acts to promote public awareness of the crucial role played by chemistry in the modern industrial environment. The BMCS is particularly active in the organisation of scientific meetings and does so in collaboration with a wide variety of other groups both within and external to the RSC. Over the past few years the BMCS has been especially active in promoting some of the important interfacial areas in which chemists are intimately involved. In recent years, it has held internationally attended meetings with the EFMC, the Society for Chemical Industry, the Society for Medicines Research and with the Biochemical Society. On average six or more scientific meetings are held each year. Support for educational activities, such as the running of lectures and day schools, and the provision of equipment are also an important component of BMCS activities. Indeed, some of these initiatives are now established as annual events. The BMCS also administers annual awards that acknowledge major scientific achievements in both academia and industry that have been carried out within the UK. The BMCS provides a significant input into Royal Society of Chemistry strategic initiatives.

3rd RSC-SCI Symposium on GPCRs in Medicinal Chemistry
(September 20-22, 2010), Schering-Plough, Oss, The Netherlands

RSC-SCI Flow Chemistry Symposium
(November 3-4, 2010), GSK, Stevenage, United Kingdom

Dr Phil JONES (Schering Plough)
Dr Stuart CAMERON (Peakdale)
Dr David ALKER (David Alker Associates)

President
Secretary
EFMC-Delegate

Impact Factor[®]:
3.150

2009 Journal Citation Reports, December 2009




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Rainer Metternich (Merck, West Point, USA)



A journal of
Chemical Publishing Societies of Europe

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Directory of Companies

An alphabetical list of pharmaceutical companies, as well as manufacturers and suppliers of products and services for medicinal chemistry in Europe

A

3M	3M Center Corporate Headquarters	ST. PAUL, MN 55144-1000	US
4SC AG	Am Klopferspitz 19a	82152 MARTINSRIED	+49 89 700763 0 DE
A & D INSTRUMENTS LTD	Abingdon Science Park	ABINGDON OX14 3YX	+44 1235 550 420 GB
AAF INTERNATIONAL BV	Egelenburg 2	1081GK AMSTERDAM	+31 20 549 44 11 NL
ABBOTT LABORATORIES	100 Abbott Park Rd	ABBOTT PARK IL 60064-3500	+1 847 937 6100 US
ABCR GmbH & Co. KG	Im Schleiert 10	76187 KARLSRUHE	49-721-95061-16 DE
ABGENE HOUSE	Blenheim Road	EPSOM SURREY KT19 AP	+44 1372 72 34 56 GB
ABSORPTION SYSTEMS	440 Creamery Way Suite 300	EXTON PA 19341	+1 610 280 7300 US
ACB BLOCKS LTD.	PO Box 10	121609 MOSCOW	+7 495 761 4365 RU
ACCELRY'S	334 Cambridge Science Park	CAMBRIDGE CB4 0WN	+44 1223 228 500 GB

American Chemical Society Publications



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pubs.acs.org
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 or 202-872-4357 (outside North America)

The American Chemical Society publishes high quality journals at the interface of chemistry, biology and medicine, including the most-cited journal in medicinal chemistry, the *Journal of Medicinal Chemistry*. In 2010 we introduce *ACS Medicinal Chemistry Letters* publishing brief communications on experimental or theoretical results of exceptional timeliness in all aspects of medicinal chemistry and its extension into pharmacology.

ACROS ORGANICS	Geel West Zone 2 Janssen Pharmaceuticaal, 3A	2440	GEEL	+32 014 57 52 11	BE
ACTIVATE SCIENTIFIC	Am Reibach 7	83209	PRIEN	+49 8051 965 16 60	DE
ACTELION	Gewerbestrasse 16	4123	ALLSCHILL	+41 61 487 45 45	CH
ACTIVE MOTIF	Avenue Franklin Roosevelt 104 Box 25	1330	RIXENSART	+32 2 653 00 01	BE
ADAMS HEALTHCARE	Lotherton Way Garforth		LEEDS LS25 2JY	+44 1132 320 066	GB
ADELPHI MANUFACTURING CO.LTD	Olympus House Mil Green Road		HAYWARDS HEATH RH16 1XQ	+44 1444 440 091	GB
ADHESIVES RESEARCH INC	400 Seaks Run Road PO BOX 100		GLEN ROCK PENNSYLVANIA 17327	+1 717 357 979	US
ADPAK MACHINERY SYSTEMS LTD	3 Pendleside Lomeshaye Industrial Estate		NELSON BB9 6RY	+44 1282 601 444	GB
AERNI-LEUCH AG/KLOCKNER	Sportweg 38	3097	LIEBEFELD/BERNE	+41 31 978 88 88	CH
AEROMATIC-FIELDER LTD	PO BOX 15		EASTLEIGH SO63 4ZD	+44 2380 267 131	GB
AFLEX HOSE LTD	Spring Bank Ind. Estate Watson Mill Lane - Sowerby Bridge		HALIFAX HX6 3BW	+44 1422 317 200	GB
AGILENT TECHNOLOGIES	Pegasus Park - De Kleetlaan 12A bus 12	1831	DIEGEM	+32 2 404 92 22	BE
AIS CLEANROOM PRODUCTS LTD	Unit 33 Riverside Medway City Estate		ROCHESTER ME2 4DP	+44 1634 719 422	GB
AKZO NOBEL NV	Velperweg 76	6824 BM	ARHNEM	+31 26 366 44 33	NL
ALCON LABS	6201 S. Freeway (T1-3)		FORT WORTH TEXAS 76134-2099		US
ALERT PRODUCTS	Hollins Lane Tilstock		WHITCHURCH SY13 3NU	+44 1948 880 627	GB
ALEXANDERWERK AG	Kippdorfsstrasse 6-24	42857	REMSCHIED	+49 219 1795 216	DE
ALFA Aesar GmbH & CO KG	Postbox 11 07 65	76057	KARLSRUHE	+49 721 84007 280	DE
ALFA LAVAL TUMBA AB	Hans Stahles vag	14780	TUMBA	+46 85 306 5000	SE
ALLERGAN INC.	P.O. Box 19534		IRVINE CA 92623	+1 714 246 4500	US
ALL-FILL INTERNATIONAL LTD	Unit 5 Gateshead Close- Sunderland Road		SANDY SG19 1RS	+44 1767 691 910	GB
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ALTRO FLOORS	Works Road		LETCHEWORTH SG6 1NW	+44 1462 480 480	GB
AMAFILTER	Kwakelkade 28 Postbus 396	1800 AJ	ALKMAAR	+31 72 527 34 00	NL
AMEC	Timothy's Bridge Road		STRATFORD UPON-AVON CV37 9NJ	+44 1789 204 288	GB
AMERSHAM PLC	Amersham Place Little Chalfont		BUCKINGHAMSHIRE HP7 9NA	+44 1494 544000	GB
AMGEN INC.	One Amgen Center Drive		THOUSAND OAKS CA 91320-1799	+1 805 447 1000	US
AMRI	Záhony u. 7	1031	BUDAPEST	+36 1 6666 132	HU
ANABIOTEC NV	Reibroekstraat 13	9940	EVERGEM	+32 9 253 60 30	BE
ANSELL OCCUPATIONAL HEALTHCARE	Wijngaardveld 34 C	9300	AALST	+32 5 371 05 05	BE
APPLESHAW ASSOCIATES	7 Ryhill Way		EARLEY RG6 RAZ	+44 1189 750 998	GB
APPLIED PRECISION INC	121 High Street		MARLBOROUGH SN8 1LZ	+44 1672 518 350	GB

APPLIKON DEPENDABLE INSTRUMENT	De Brauwweg 13 PO BOX 149		SCHIEDAM	+31 10 462 18 55	NL
ARGENTA DISCOVERY LTD	8/9 Spire Green Centre Flex Meadow	3100 AC	HARLOW ESSEX CM19 5TR	+44 1279 485 674	GB
ARMFIELD LTD	Bridge House West Street		RINGWOOD BH24 1DY	+44 1425 478 781	GB
ARQUEL	19 Presidential Way		WOUBURN MA 01801-5140	+1 781 994 0300	US
ARRAY BIOPHARMA	3200 Walnut Street		BOULDER CO 80301	+1 303 381 6645	US
ASTEX TECHNOLOGY LTD	250 Cambridge Science Park Milton Road		CAMBRIDGE CB4 0WE	+44 1223 226 200	GB
ASTON SCIENTIFIC LTD	Silverdales House 111 Wendover Road		STOKE MANDEVILLE HP22 5TG	+44 1296 614 144	GB
ASTRA ZENECA PLC	15 Stanhope Gate		LONDON W1K 1LN	+44 (0)20 7304 5000	GB
ASYNT LT	Unit 29 Hall Barn Road Industrial Estate		ISLEHAM CB7 5RJ	+44 (0)1638 783614	GB
ATLAS MATERIAL TESTING TECHNOLOGY BV	Aalsvoort 69 PO BOX 182 (7241 MA)		LOCHEM	+31 57 325 64 65	NL
AUTODOSE SA	18 Chemin des Aulx	7240 AD	GENEVA	+41 22 884 13 30	CH
AVENTIS PHARMACEUTICALS INC.	300 Somerset Corporate Boulevard	1228	BRIDGEWATER NJ 08807-2854	+1 800 981 2491	US
AVERY BERKEL	Foundry Lane		SMETHWICK B66 2LP	+44 8709 050 064	GB
B. BRAUN MEDICAL	Carl-Braun-Straße 1		MELSUNGEN	+49 (0) 56 61 71-0	DE
B.R.S.	Steenweg op Ruysbroek 290	34212	DROGENBOS	+32 2 3342270	BE
BASF AG	Carl-Bosch-Straße 38	1620	LUDWIGSHAFEN	+49 (0)621 60-0	DE
BAYER AG	Kaiser Wilhelm Allee 1	67056	LEVERKUSSEN	+49 (0)214 301	DE
BCH LTD	Spring Place Millfold	51373	WHITWORTH OL L2 8DN	+44 1706 852 122	GB
BO BIOSCIENCES BENELUX	POB 13 - Erebodegem-Dorp 86	9320	EREMBODEGEM	+32 53 720 600	BE
BEAUFOUR IPSSEN INTERNATIONAL SNC	37 rue Spontini	75116	PARIS	+33 2 37 62 89 00	FR
BEECHWOOD RECRUITMENT LTD	221 High Street		LONDON W3 9BY	+44 2039 928 647	GB
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marketing@bentham.org
www.bentham.org



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BIOFOCUS A GALAPAGOS CO DPI	Chesterford Research Park Saffron Walden		ESSEX CB10 1XL	44 1 799 533 588	GB
BIOGAEA FERMENTATION AB	PO Box 965	22009	LUND	+46 46 280 1700	SE
BIOMEN INC	14 Cambridge Center		CAMBRIDGE MA 2142	+1 617 679-2000	US
BIOMENEX	4600 Norris Canyon Road		SAN RAMON, CA 94583	+1 925 275 0550	US
BIOGLAN LABORATORIES LTD	North Way Walworth Industrial Estate		ANDOVER SP10 5AZ	+44 1264 363 117	GB
BIOIBERICA SA	Plaza Francisc Macia 7	8029	BARCELONA	+34 93 490 4908	ES
BIOLINE UK INC	16 The Edge Business Centre Humber Road		LONDON NW2 6EW	+44 2088 305 300	GB
BIOMATECH SA	Zone Industrielle de l'Ision - 115 Rue Pasteur	38670	CHASSE-SUR-RHONE	+33 4 78 07 92 34	FR
BIOPHARMA PROCESS SYSTEMS	Biopharma House Winnall Valley Road		WINCHESTER SO23 0CD	+44 1962 841 092	GB
BIOQUELL PHARMA	Walworth Road		ANDOVER SP10 5AA	+44 1264 835 853	GB
BIO-RAD LABORATORIES	Fokkerstraat 10	3905 KV	VEENENDAAL	+31 31 854 06 66	NL
BIORELIANCE LTD	Innovation Park Hillfoots Road		STIRLING FK9 4NF	+44 1786 451 318	GB
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