

# XVIIth International Symposium on Medicinal Chemistry

Barcelona, Spain  
1 - 5 September 2002



FINAL PROGRAMME



European Federation for Medicinal Chemistry



Sociedad Española de Química Terapéutica

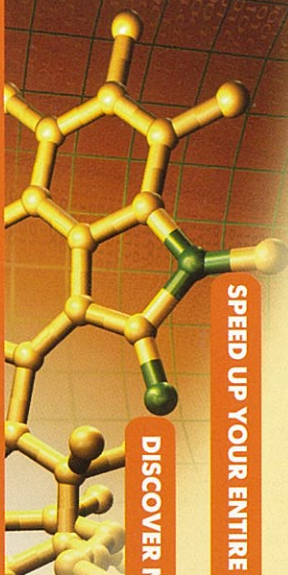




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MEDICINAL CHEMISTRY, SEPTEMBER 1-5, 2002, BARCELONA, SPAIN**

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## WELCOME

*Dear Colleagues,*

*On behalf of the Organising Committee of the XVIth International Symposium on Medicinal Chemistry, I cordially welcome you to Barcelona and to this scientific event.*

The International Symposia on Medicinal Chemistry are key scientific events that, since the sixties have been organised every two years in different cities of Europe. They have an attractive multidisciplinary scope and worldwide attendance from both industry and academia. The present edition offers a Scientific Programme covering the hottest techniques and domains of drug discovery.

The Congress venue, Palau de Congressos de Barcelona, is located in the central area of Barcelona and offers modern facilities for speakers, exhibitors and attendants.

Barcelona is a modern economically active metropolis with almost four million inhabitants. Barcelona is also a tourist city especially famous for its gothic and modernist monuments. Gaudi's buildings and the Picasso Museum are internationally well known. Barcelona offers other tourist attractions like artistic events, shopping areas, rich gastronomy and interesting natural and monumental surroundings.

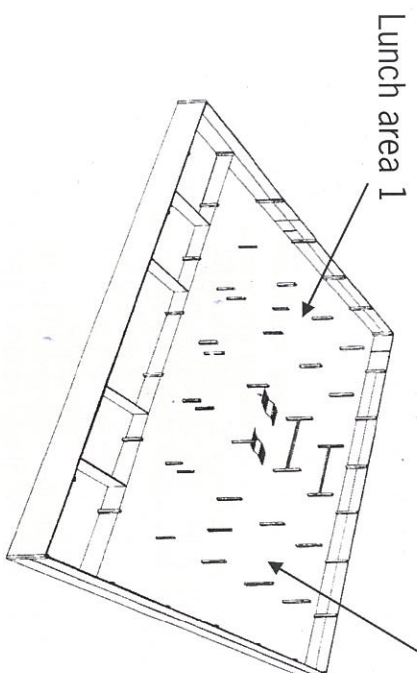
*Looking forward to your satisfaction and active participation,*

**Ferran Sanz**  
Chairman

## CONGRESS VENUE

level 0

Commercial Exhibition and poster area

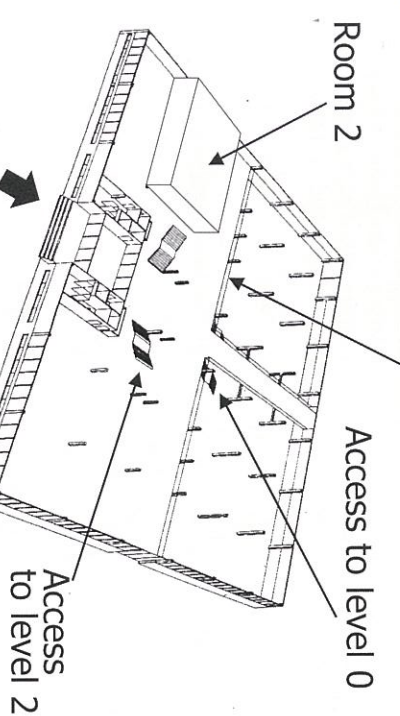


level 1

Secretariat desk

Room 2

Access to level 0



Main entrance

Access  
to level 2

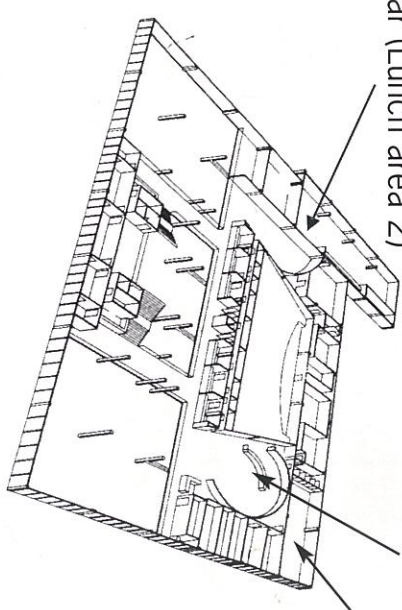
## CONGRESS VENUE

level 2

Presentation preview

Snack bar (Lunch area 2)

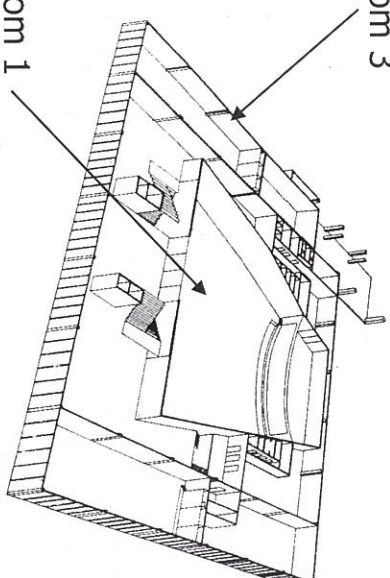
Room 4



level 3

Room 3

Room 1





## KEY INFORMATION FOR ALL ATTENDANTS

- The Symposium is divided into three parallel sessions. The second figure in the session number corresponds to the room where it will be held. For instance, Session X.2 is held in room 2. (Please see enclosed maps of the Venue)
- Some lectures will be video recorded and made available through Internet from Monday, September 16 at the following addresses:  
[www.opex.com/17ismc](http://www.opex.com/17ismc)  
[www.prous.com](http://www.prous.com)  
[www.imim.es/grlb](http://www.imim.es/grlb)
- Posters will be displayed during the whole Symposium time at level 0. Author/s will be present during the corresponding session. (See Symposium programme and posters list)
- A large Commercial Exhibition can also be visited at level 0.
- There will be free access to Internet at the Cyber Corner located in the exhibition area.
- A buffet lunch will be served every day from 13:00 to 14:00 at levels 0 and 2. A ticket for each lunch is included in your envelope. The hostesses will ask for it at the entrance of the lunch area.
- Coffee breaks will be served in the Commercial Exhibition area every day from 10:40 to 11:20 and on Monday and Wednesday evening from 15:50 to 16:20.
- On Sunday, September 1, after the Opening Lecture, a welcome cocktail will be served to all attendants and their accompanying persons at level 1 (main entrance).
- On Monday, September 2 at 20:30, all attendants and their accompanying persons are cordially invited to the Concert that will be celebrated at the Basilica of Santa Maria del Mar.
- The Gala Dinner will be celebrated on Wednesday, September 4 at the Hotel Fira Palace. This is an optional dinner. Tickets will be on sale at the Secretariat Desk until Monday September, 2 (Price: 75 €). A vegetarian menu will be available on request made before Monday September, 2 at 18:00.
- As in all major and tourist cities, some areas in Barcelona may be visited by pickpockets. There is no significant risk for your personal and physical security but we recommend that you pay attention to your belongings, carrying for instance your handbag always closed and under control and leaving your documents and valuable objects at your hotel. If you are travelling with your own car, do not leave valuable belongings inside when it is parked in the street.

## KEY INFORMATION FOR SCIENTIFIC PRESENTATIONS

### ***If you are session chairperson...***

All Symposium chairpersons are asked to be at the room where the session will be held 15' in advance of the beginning of the session to meet with speakers.

There are two speech formats:

- 50' lectures divided into 40' presentation and 10' discussion
- 25' oral communications divided into 20' presentation and 5' discussion

The chairpersons are earnestly asked to strictly follow the scheduled times for the speeches in order to facilitate the attendance shift from one session to another. For the same reason, no changes to the order of the presentations is allowed. Time has to be kept free if a speaker happens to be missing.

### ***If you are speaker...***

All speakers are asked to be at the room where the session will be held 15' in advance of the beginning of the session, regardless of the particular time of their speech. Once in the room, they must contact the session chairperson and the technician in charge of projection.

The standard format for presentations is MS-PowerPoint (95, 97 or 2000). Please use the "embedded fonts" option to avoid certain problems when projecting files prepared on a different computer. Authors can carry their projections on MS-Windows formatted CD-ROMs or 3.5" diskettes, or on their own laptop, which will be connected to a beamer provided by the organisation.

Classical slides or overhead transparencies could be accepted upon request if made at the beginning of the congress at the Symposium Secretariat.

A preview room for presentations is available during the Symposium. It is located on level 2 and will be open throughout the Symposium.

For any request, please feel free to contact the organisation staff at the Secretariat Desk located at level 1 (main entrance)

### ***If you present a poster...***

All posters should be displayed during the whole Symposium time at level 0. Each poster has been scheduled in one of four poster sessions to assure the presence of the author/s besides their poster during at least a one-hour period. The four poster sessions are:

- Poster session A, Monday, September 2, 14:00-15:00 (from P.101 to P.214)
- Poster session B, Tuesday, September 3, 14:00-15:00 (from P.215 to P.321)
- Poster session C, Wednesday, September 4, 14:00-15:00 (from P.323 to P.435)
- Poster session D, Thursday, September 5, 11:10-12:10 (from P.436 to P.556)

Please see the alphabetically ordered list of posters in this programme for the code and session assigned to your poster.

Appropriate elements for fixing the posters to the wall will be available at the Secretariat Desk. No pins can be used.



## SCIENTIFIC PROGRAMME

Sunday, September 1, 2002

## Opening lecture

## Room 1

**Chairperson: Ferran Sanz. IMIM, Universitat Pompeu Fabra, Barcelona (Spain).**

19:00-19:40 Membrane protein targets for medicinal chemistry: mechanistic insights into cell signaling from structure-function elucidation.

Harel Weinstein. Mount Sinai School of Medicine, New York (USA).

Monday, September 2, 2002

## Session 1.1. GPCR (I)

## Room 1

**Chairperson: Harel Weinstein. Mount Sinai School of Medicine, New York (USA)**9:00-9:50 Trying to understand mechanisms of action of G protein coupled receptors.  
Philip G. Strange. University of Reading (UK).9:50-10:40 Designing receptors and ligands in 7TM G protein coupled receptors.  
Thue W. Schwartz. Panum Institute (Denmark).

## Session 1.2. Development of chemical libraries

## Room 2

**Chairperson: Hugo Kubinyi. University of Heidelberg (Germany).**9:00-9:50 From protein domains to drugs: natural products as guiding principles for compound library development.  
Herbert Waldmann. Max-Planck-Institut für Molekulare Physiologie, Dortmund (Germany).9:50-10:15 Strategy for the optimised production of tertiary amine libraries.  
Angus R. Brown. Organon Laboratories Ltd. (UK).10:15-10:40 Focused library of potential serine protease inhibitors.  
Stanley A. Lang. Chemical Diversity Labs, Inc. (USA).

## Session 1.3. Kinases

## Room 3

(session organised by the Med. Chem. Div. of ACS)

**Chairperson: Patrick M. Woster. Wayne State University, Detroit (USA)**9:00-9:25 Discovery of novel inhibitors of tyrosine kinases via a targeted combinatorial library pharmacophore approach.  
Thomas R. Webb. ChemBridge Corp. and CRL (USA).9:25-9:50 Pyrazolo[3,4-d]pyrimidines as orally active Lck inhibitors.  
Gavin Hirst. Abbott Bioresearch Center (USA).

## SCIENTIFIC PROGRAMME

9:50-10:15 Evaluation of the tyrosine kinase domain of Tyk2 as a potential drug target.  
Kristin Tøndel. Norwegian University of Science and Technology (Norway).10:15-10:40 Homology modelling and docking studies on Varicella Zoster virus thymidine kinase.  
Loredana Spadola. Università di Napoli (Italy).

10:40-11:20 Coffee Break (Level 0)

## Session 2.1. GPCR (II)

## Room 1

**Chairwoman: María Luz López Rodríguez. Universidad Complutense de Madrid (Spain).**11:20-12:10 Histamine receptors, a place where medicinal chemistry of the past and the future meet.  
Henk Timmerman. Leiden/Amsterdam Center for Drug Research (The Netherlands).12:10-13:00 Recent developments in the field of adenosine receptor ligands.  
Pier Giovanni Baraldi. Università di Ferrara (Italy).

## Session 2.2. Cardiovascular Diseases

## Room 2

**Chairperson: Fulvio Gualtieri. Università di Firenze (Italy).**11:20-11:45 Hit finding strategies towards urotensin II receptor antagonist.  
Stefanie Flohr. Aventis Pharma Deutschland GmbH (Germany).11:45-12:10 Discovery of selective CYP11B2 (aldosterone synthase) inhibitors for the therapy of congestive heart failure and myocardial fibrosis.  
Rolf Hartmann. Saarland University (Germany).12:10-12:35 Synthesis, SAR, eADME-profiling and pharmacological results of novel  $I_{Ks}$  channel blockers.  
Uwe Gerlach. Aventis Pharma Deutschland GmbH (Germany).12:35-13:00 Modelling an allosteric binding site of the  $M_2$  muscarinic acetylcholine receptor.  
Kirstin Jöhren. Heinrich-Heine-Universität Düsseldorf (Germany).

## Session 2.3. Hot topics in drug discovery and development

## Room 3

**Chairperson: Gerhard F. Ecker. University of Vienna (Austria).**11:20-12:10 Structure and function of orphan nuclear receptors.  
Timothy M. Wilson. GlaxoSmithKline (USA).12:10-12:35 The first orally active low molecular weight agonists for the LH receptor: thienopyrimidines with therapeutic potential.  
Nicole C. R. van Straten. N.V. Organon (The Netherlands).12:35-13:00 Targeted lysosome disruptive elements for the improvement of cell specific drug delivery.  
Sabine M. W. van Rossenberg. Leiden/Amsterdam Center for Drug Research (The Netherlands)



## SCIENTIFIC PROGRAMME

## 14:00-15:00 Poster session A

Level 0

## 15:10-15:50 Plenary lecture of the Nauta Awardee

Room 1

**Chairperson: Henk Timmerman. Leiden/Amsterdam Center for Drug Research (The Netherlands).**

Structure and activity revisited – Property spaces and emergent meaning.  
Bernard Testa. Université de Lausanne (Switzerland)

15:50-16:20 Coffee Break (Level 0)

## Session 3.1. Organic chemistry in drug development (I)

Room 1

**Chairperson: Helmut Buschmann. Esteve SA, Barcelona (Spain).**

16:20-17:10 Molecules to market: The challenges for chemical development.  
Peter Spargo. Pfizer (UK).

17:10-17:35 Enhanced chromatographic resolution of derivatized alcohol intermediates of biologically active compounds.

Yves Leblanc. Merck Frosst Centre for Therapeutic Research (Canada).

17:35-18:00 New approaches in the development of orally bioavailable selective group 2 metabotropic glutamate receptor agonists.

Concepción Pedregal. Lilly, SA (Spain).

## Session 3.2. GPCR (III)

Room 2

**Chairperson: Roberto Pellicciari. Università di Perugia (Italy).**

16:20-17:10 Reclassification of G-protein Coupled Receptors using thematic analysis.  
Martin J. Slater. BioFocus plc, Sittingbourne Research Centre (UK).

16:45-17:10 R107500. A new 5-HT<sub>2A/2C</sub> antagonist with potential anxiolytic profile.  
J. Ignacio Andrés. Janssen-Cilag (Spain).

17:10-17:35 Conformationally constrained aminobutyrophenones as new 5-HT<sub>2</sub> ligands. Synthesis, molecular modelling and assays as antagonists and inverse agonists.  
Enrique Raviña. Universidade de Santiago de Compostela (Spain).

17:35-18:00 Impact of the aryl substituent kind and distance from pyrimido [2,1-f]purindiones on the adenosine receptor selectivity and antagonistic properties.  
Katarzyna Kiec-Kononowicz. Jagiellonian University Medical College (Poland).

## Session 3.3. Metabolic diseases

Room 3

**Chairperson: Rolf W. Hartmann. Saarland University (Germany).**

16:20-16:45 Novel imidazolines as potent glucose-dependant stimulators of insulin secretion without activity on the K<sub>ATP</sub> channel.

Palle Jakobsen. Medicinal Chemistry Research (Denmark).

## SCIENTIFIC PROGRAMME

16:45-17:10 Selective inhibitors of the 11 $\beta$ -hydroxysteroid dehydrogenase type I (11 $\beta$ -HSD1). A new class of potential anti-diabetic drugs.  
Tjeerd Barf. Biovitrum AB (Sweden).

17:10-17:35 Discovery of potent selective antagonists of the human melanin-concentrating hormone receptor 11Cby.  
David R. Witty. GlaxoSmithKline (UK).

17:35-18:00 The discovery of A-151892: A novel bladder selective K<sub>ATP</sub> channel opener.  
Sean C. Turner. Abbott Laboratories (USA).



## SCIENTIFIC PROGRAMME

Tuesday, September 3, 2002

## Session 4.1. Early ADMET (I)

Room 1

**Chairperson: Gabriele Cruciani. Molecular Discovery Ltd. (UK) & Università di Perugia (Italy).**

- 9:00-9:50 Property-based design: Getting the ADME properties fast and right.  
Han van de Waterbeemd. Pfizer Global Research and Development (UK).
- 9:50-10:15 Rapid prediction of blood-brain distribution of drugs with aqueous two-phase partitioning and HPLC or octanol-buffer partitioning.  
Boris Zaslavsky. Analiza Inc. (USA).
- 10:15-10:40 Biological monitoring of xenobiotics by high-throughput immunochemical techniques. Mikaela Nickkova. IIQAB-CSIC (Spain).

## Session 4.2. Cancer (I)

Room 2

**Chairperson: Carmen Avedaño. Universidad Complutense de Madrid (Spain).**

- 9:00-9:25 Molecular mechanisms of resistance to imatinib, a tyrosine kinase inhibitor: A molecular dynamics study.  
Leonardo Scapozza. ETH, Zurich (Switzerland).
- 9:25-9:50 Fuzzy Logic based Focused Libraries (FL/FL) for HTS screening: Application to anti-carcinogenic compounds.  
Jacques R. Chrétien. University of Orléans (France).
- 9:50-10:15 A new class of exceptionally potent DNA cross-linking agents.  
Moana Tercei. Auckland Cancer Society Research Centre. University of Auckland (New Zealand).
- 10:15-10:40 Alkylating agents from sugars. Synthesis of cyclophosphamides derived from glycosyl glycerols. Felipe Alcudia. Universidad de Sevilla (Spain).

## Session 4.3 Pulmonary diseases

Room 3

**Chairperson: Hamish Ryder. Almirall Prodesfarma SA, Barcelona (Spain).**

- 9:00-9:25 Potent inhibitors of lge synthesis in human B-lymphocytes: From a peptidomimetic lead to orally active drug candidates.  
Peter Eitmayr. Novartis Forschungsinstitut (Austria).
- 9:25-9:50 Identification and optimisation of non-redox inhibitors of 15-lipoxygenase-a.  
Alan Brown. Pfizer (UK).
- 9:50-10:15 The design and synthesis of a novel series of dual acting molecules possessing 5-lipoxygenase enzyme inhibition and histamine H1 receptor antagonist properties. Ralph T. Scannell. UCB Research, Inc. (USA).
- 10:15-10:40 A novel orally active inhibitor of HLE.  
Marton Varga. Chinoin Pharmaceutical and Chemical Works Co. Ltd. (Hungary)
- 10:40-11:20 Coffee Break (Level 0)

## SCIENTIFIC PROGRAMME

## Session 5.1. Cancer (II)

Room 1

**Chairwoman: María Isabel Fernández (Spain)**

- 11:20-12:10 Development of novel anti-herpes compounds: potential application in combined gene/chemotherapy of cancer.  
Jan Balzarini. Katholieke Universiteit Leuven (Belgium).
- 12:10-12:35 SDZ LAV 694: A novel antiproliferative agent for topical use.  
Peter Nussbaumer. Novartis Forschungsinstitut (Austria).
- 12:35-13:00 Antitumor activity of podophylotoxin D-ring analogue derivatives  
Claude Monneret. Institut Curie (France).

## Session 5.2. Phosphodiesterases and phospholipases

Room 2

**Chairperson: Graham Warwellow. Almirall Prodesfarma SA, Barcelona (Spain).**

- 11:20-12:10 Discovery of highly potent and well tolerated PDE4 inhibitors.  
Yves Girard. Merck Frosst Centre for Therapeutic Research (Canada).
- 12:10-12:35 New xanthine-based PDE5 inhibitors.  
Bernat Vidal. Almirall Prodesfarma SA (Spain).
- 12:35-13:00 Inhibitors of phosphopantetheine adenylyltransferase (PPAT).  
Lihua Zhao. PanTherix Ltd. (UK).

## Session 5.3. GPCR: Cannabinoid receptors

Room 3

**Chairperson: Marcel Hibert. Université de Strasbourg (France).**

- 11:20-12:10 Cannabinoid proteins as therapeutic targets.  
Alexandros Makriyannis. University of Connecticut (USA).
- 12:10-12:35 New approaches for psychosis and obesity treatment: design, synthesis and SAR of 3,4-diarylpyrazolines as potent, selective and orally active cannabinoid CB<sub>1</sub> receptor antagonists.  
Jos H. M. Lange. Solvay Pharmaceuticals (The Netherlands).
- 12:35-13:00 Design, synthesis and biological evaluation of new endocannabinoid transporter inhibitors.  
Silvia Ortega-Gutiérrez. Universidad Complutense de Madrid (Spain).

## 14:00-15:00 Poster session B

Level 0

## 15:00-16:30 Round table on Patentability

Room 2

**Chairperson: Israel Agranat. The Hebrew University of Jerusalem (Israel)**

- Reporters:
- Robert E. Perry, Gill, Jennings & Every (UK)
- Per Lindberg, AstraZeneca (Sweden)
- Israel Agranat, The Hebrew University of Jerusalem (Israel)



## SCIENTIFIC PROGRAMME

Wednesday, September 4, 2002

## Session 6.1. CNS (I)

Room 1

**Chairperson: Hans-Dieter Höltje. Heinrich-Heine-Universität Düsseldorf (Germany).**

9:00-9:50 Molecular pathway of neurodegeneration: new treatment opportunities.  
Jörg B. Schulz. University of Tübingen (Germany).

9:50-10:15 Binding models of reversible inhibitors to monoamine oxidases.  
Antonio Carrieri. Università di Bari (Italy).

10:15-10:40 Design, synthesis and SAR of PARP-1 inhibitors.  
Vincent Kalish. Guilford Pharmaceuticals Inc. (USA).

## Session 6.2. Early ADMET (II)

Room 2

**Chairperson: Wolfgang Guba. F. Hoffmann-La Roche Ltd., Basel (Switzerland).**

9:00-9:50 DMPK-based de novo ligand design.  
Gabriele Cruciani. Molecular Discovery Ltd. (UK) & Università di Perugia (Italy).

9:50-10:15 Similarity-Based Structure-Activity Relationship (SIBAR) as tool for early ADMET profiling.  
Gerhard F. Ecker. University of Vienna (Austria).

10:15-10:40 Early ADME assessment by Adaptive Fuzzy Partitioning (AFP).  
Marco Pintore. BioChemics Consulting & University of Orléans (France).

## Session 6.3. Third world diseases

Room 3

(Session organised by the Med. Chem. Div. of ACS)

**Chairperson: Patrick M. Woster. Wayne State University, Detroit (USA)**

9:00-9:25 Potent, parasite targeted akylopyramine analogues.  
Patrick M. Woster. Wayne State University (USA)

9:25-9:50 Antimicrotubule antiparasitic activity of novel dinitro aniline sulfonamides  
Karl Werbovetz. Ohio State University. (USA).

9:50-10:15 Leishmaniasis: chemotherapy and modulators of MDR.  
Angel G. Ravelo Instituto Universitario de Bio-Organica (Spain).

10:15-10:40 Exploitation of parasite heme metabolism by xanthenes.  
Michael Riscoe. Medical Research Service, VA Medical Center (USA)

10:40-11:20 Coffee Break (Level 0)

## SCIENTIFIC PROGRAMME

## Session 7.1. New methods and technologies in drug discovery (I)

Room 1

**Chairperson: Angelo Carotti. Università di Bari (Italy)**

11:20-12:10 Gene targeted mice as models for drug discovery.  
Mariano Barbacid. Centro Nacional de Investigación Oncológica, Madrid (Spain).

12:10-12:35 Many needles in a haystack: A stochastic search from protein sequence to drug design.  
Amiram Goldblum. University of Jerusalem (Israel).

12:35-13:00 Receptor-based 3D-QSAR: An interesting tool for drug design.  
Wolfgang Sippl. Heinrich-Heine-University of Düsseldorf (Germany).

## Session 7.2. CNS (II)

Room 2

**Chairperson: Wolfgang Froestl. Novartis Pharma AG (Switzerland).**

11:20-11:45 Dihydropyridine neuropeptide  $\gamma$   $\gamma_1$  receptor antagonists: cyanoguanidine-linked derivatives with improved oral bioavailability.  
Graham S. Poindexter. Pharmaceutical Research Institute (USA).

11:45-12:10 Synthesis and structure-activity studies on alkylated analogues of the partial GABA<sub>A</sub> agonist 4-PIOL.  
Bente Frølund. The Royal Danish School of Pharmacy (Denmark)

12:10-12:35 Synthesis and biological evaluation of  $\beta$ -aminosulfones as novel NMDA-NR1/2B subtype selective antagonists.  
Georg Jaeschke-F. Hoffmann-La Roche (Switzerland)

12:35-13:00 Molecular determinants for metabotropic glutamate receptor activation and blockade. Molecular dynamics and electrostatic potential analysis studies.  
Gabriele Costantino Università di Perugia (Italy)

## Session 7.3. Antibiotics

Room 3

**Chairwoman: María Teresa García. Instituto de Química Médica, CSIC, Madrid (Spain).**

11:20-12:10 Do we need new antibiotic resistance mechanisms?  
Patrice Courvalin. Institut Pasteur, Paris (France).

12:10-12:35 The DeNovo design of chimeric lipid-peptide substrates and time dependent inhibitors for the *Staphylococcus aureus* signal peptidase SpsB.  
Gordon Bruton. GlaxoSmithKline (UK).

12:35-13:00 Novel antibiotics derived from TAN 1057 A,B for the treatment of MRSA infections.  
Michael Brands. Bayer AG (Germany).

14:00-15:00 Poster session C

Level 0



## SCIENTIFIC PROGRAMME

## 15:10-15:50 Plenary lecture of the UCB Awardee

Room 1

**Chairperson: Edmond Differding. UCB (Belgium)**

- Case study: Gleevec – A new treatment modality for chronic Myelogenous Leukemia.  
 Juerg Zimmermann, Novartis Pharma AG (Switzerland)  
 15:50-16:20 Coffee Break (Level 0)

**Session 8.1. Organic chemistry in drug development (II)**

Room 1

**Chairperson: Robin Ganellin. University College London (UK).**

- 16:20-17:10 Asymmetric synthesis made simple: Discovery of novel reactivity leading to practical processes.  
 Erick M. Carreira, ETH, Zürich (Switzerland).  
 17:10-17:35 NMDA-NR2B subtype selectivity of stereoisomeric 2-(1,2,3,4-tetrahydro-1-isoquinolyl)ethanol derivatives.  
 Klaus Th. Wanner, Universität München (Germany).  
 17:35-18:00 Semi-synthesis and activity of pacitaxel analogues.  
 Arturo Battaglia, Istituto CNR "I.S.O.F.", Bologna (Italy).

**Session 8.2. New methods and technologies in drug discovery (II)**

Room 2

**Chairperson: M. Fethi Sahin. Gazi University of Pharmacy, Ankara (Turkey).**

- 16:20-16:45 Accelerated drug design using high throughput protein X-ray crystallography.  
 Martyn Frederickson, Astex Technology (UK).  
 16:45-17:10 Structure, selectivity, and the promise of high-throughput X-Ray crystallography in the future of medicinal chemistry.  
 Jeff Blaney, Structural Genomix (USA).  
 17:10-17:35 How to acquire new biological activities in old compounds by computer prediction.  
 Vladimir V. Porokhov, V.N. Orekhovich Institute of Biomedical Chemistry of RAMS (Russia).  
 17:35-18:00 Non-peptide spacers replace intervening amino acids in the ITAM sequence binding to Syk tandem SH2 domain.  
 Nico J. de Mol, Utrecht University (The Netherlands).

**Session 8.3. Antivirals (I)**

Room 3

**Chairperson: Maria José Camarasa. Instituto de Química Médica, CSIC (Spain).**

- 16:20-17:10 Antiviral drug discovery. Chris McGuigan, University of Wales (UK).  
 17:10-17:35 New anti-HIV drug candidates: Diaryltriazines, diarylpyrimidines and diaminopyrimidines.  
 Chih Y. Ho, Johnson & Johnson (USA).  
 17:35-18:00 HCV NS3 protease inhibitors: Novel antiviral agents for future treatment of hepatitis C virus infections.  
 Montse Llinàs-Brunet, Boehringer Ingelheim Ltd. (Canada).

## SCIENTIFIC PROGRAMME

## Thursday, September 5, 2002

**Session 9.1. New methods and technologies in drug discovery (III)**

Room 1

**Chairperson: Jordi Quintana. Laboratorios Dr. Esteve SA (Spain).**

- 9:10-10:00 Bioinformatics approaches to the deciphering of protein interaction networks.  
 Alfonso Valencia, Centro Nacional de Biotecnología (CSIC), Madrid (Spain).  
 10:00-10:25 Identification of "latent hits" in compound screening collections.  
 Jordi Mestres, Organon Laboratories Ltd. (Scotland).  
 10:25-10:50 Distant collaboration in drug discovery: The LINK3D project.  
 Manuel Pastor, GRIB (IMIM/UPF), Barcelona (Spain).

**Session 9.2. Pain and inflammation**

Room 2

**Chairperson: Albert Palomer. Ferrer Group, Barcelona (Spain).**

- 9:10-10:00 NO-releasing drugs, a new class of anti-inflammatory agents.  
 Piero del Soldato, NicOx S.A. (France).  
 10:00-10:25 Vanilloid receptor antagonists: structure activity relationships via parallel and targeted synthesis.  
 Nicholas I. Carruthers, Johnson & Johnson (USA).  
 10:25-10:50 Inhibitors of glutamate carboxypeptidase II - Novel neuroprotective therapeutics.  
 Pavel Majer, Guilford Pharmaceuticals Inc. (USA).

**Session 9.3. Antivirals (II)**

Room 3

**Chairperson: Jan Balzarini. Katholieke Universiteit Leuven (Belgium).**

- 9:10-10:00 The quest for small ligands acting at viral chemokine receptors.  
 Rob Leurs, Leiden/Amsterdam Center for Drug Research (The Netherlands).  
 10:00-10:25 The design and development of potent, non-peptidic inhibitors of hepatitis C protease.  
 David M Andrews, GlaxoSmithKline (UK).  
 10:25-10:50 Discovery of novel non-covalent inhibitors of the hepatitis C virus serine protease.  
 Frank Nargies, IRBM - MRL, Rome (Italy).  
 10:50-11:20 Coffee Break (Level 0)

**11:10-12:10 Poster session D**

Level 0

**Closing lecture**

Room 1

**Chairperson: Ferran Sanz. IMIM-Universitat Pompeu Fabra, Barcelona (Spain).**

- 12:10-13:00 Challenges in drug discovery in the XXIst Century: Initiatives of the European Union.  
 Alfredo Aguilar, Directorate General Research, European Commission, Brussels (Belgium).



## SATELLITE SESSIONS

These sessions are initiatives of companies participating in the Commercial Exhibition that aim to present the characteristics of their products and scientific topics related with them.

### Tuesday, September 3

#### **Knowledge management challenges in drug discovery (Prous Science) Room 3**

15:00 - 16:30

Today's drug discovery and development community faces the challenge of analyzing the abundance of information generated by scientific activities. In fact, it is predicted that more information will be generated in the next two years than in the whole history of biomedical research. The acquisition, analysis and prediction of biomedical information is therefore crucial for successful advances in the field.

The presentations included in this satellite symposium:

- \* Recent supercomputation advances in biomedical research
- \*\* Integrated approach to the retrieval, analysis and prediction of biomedical data
- \*\* Discovery of new therapeutic targets using high-throughput functional genomics will demonstrate from several perspectives innovative solutions for managing the ever-increasing data resulting from the information era.

Since 1958, Prous Science has been providing the best and most progressive new ways to present and discuss drug and medical information. By organizing this satellite symposium, Prous continues its long-standing commitment of knowledge dissemination and management for a healthier world.

#### **Focused Lead Desing Workshop (Accelrys)**

**Room 4**

15:00 - 16:00

Discovery Studio MedChem Explorer enables medicinal chemists to design active compounds faster using an *in silico* approach without causing the researcher to spend a lot of time learning an "expert" modeling application. From a desktop PC, this Windows application offers chemists an intuitive interface that provides enterprise-wide access to industry leading methods for pharmacophore modeling, conformation analysis, property calculation, ADME prediction, biological activity prediction, and more. Examples of using DS MedChem Explorer during compound design and lead optimization will be shown.

## SATELLITE SESSIONS

### Wednesday, September 4

#### **Chemical Computing Group**

**Room 2**

13:45 - 14:15

Chemical Computing Group, a leading provider of state-of-the-art discovery software, delivers enterprise-wide solutions to pharmaceutical and biotech researchers worldwide.

It will be hosting a presentation/workshop on Wednesday, Sept. 4, 2002 at 13:45 in Room 2, 2002 highlighting the use of MOE, the Molecular Operating Environment, by the medicinal chemistry community. MOE is the first drug discovery software package of its kind that is accessible to a range of researchers including methods developers, computational experts and medicinal chemists. The capability for computational experts and method developers to share their ideas and algorithms with the medicinal group makes it the ideal vehicle for corporate wide drug research & development.

Medicinal chemists are able to access the power of MOE's discovery applications through a choice of entry points such as their home-grown intranet web page, the MOE/Web interface or focused native MOE interfaces customized in the MOE programming language. In addition, MOE's platform independence (Windows, Linux, Unix) provides a cost effective hardware environment for all researchers concerned.

The presentation/workshop will take attendees through a variety of ways MOE is presently being used by industrial medicinal chemists including Protein modeling, QSAR, conformational search, etc. As part of the workshop, there will be a live demonstration featuring practical examples of these applications.

CCGs is located at Booth #32 in the exhibition hall.



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New xanthine derivatives as adenosine receptor antagonists	Akgün	P103
Roles of DNA topoisomerase II $\alpha$ in the cell cycle regulation of mouse embryonic cells at the early stage of development	Akimitsu	P104
Enantioselective synthesis of (E)-aryl vinyl sulfoxides. Putative antimalarial drugs	Alcudia	P105
Pyrazolo[3,4-b]quinoxalines. a new class of cyclin-dependent kinases inhibitors	Aldana	P106
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Synthesis and antimicrobial activity of 4-Carbethoxymethyl-2-[(N,N-disubstituted thiocarbamoylthio)acylamino]thiazoles	Altintas	P111
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Phenylcarbamates and cholinesterases: synthesis and in vitro evaluation as ligands for nicotinic acetylcholine receptors (nAChRs)	Andră	P113
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Synthesis and anti-MDR activity of arylmethylene derivatives of the pyrazino [2,1-b]quinazoline-3,6-dione system	Avendaño	P124
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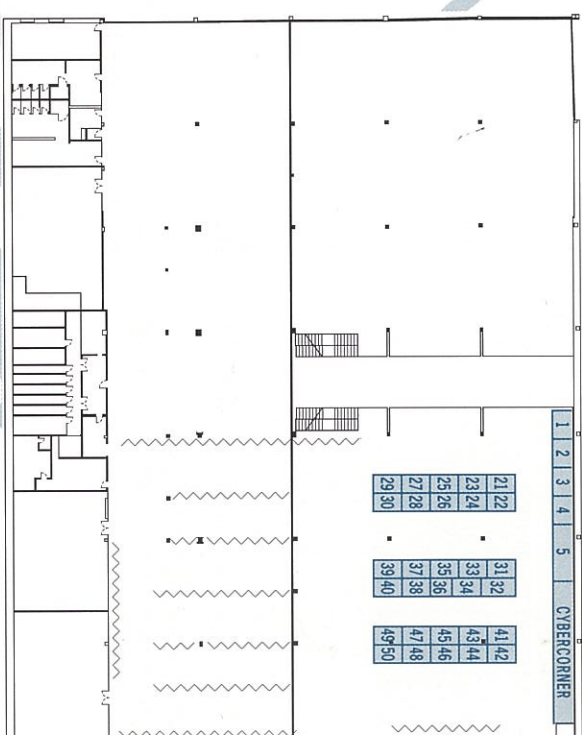
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## COMMERCIAL EXHIBITION

A wide exhibition area is available at level 0 where posters will also be presented. The exhibition will be opened from Sunday September, 1 to Thursday September, 5.

## Exhibition Floorplan





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See the power of integrity for yourself! Attend on September 3<sup>rd</sup>, 3-4:30 p.m., the Prous Science Satellite Symposium, *Next-Generation Knowledge Management Tools for Drug R&D and Clinical Medicine*, part of the 17th International Symposium on Medicinal Chemistry. For more details, and to register, visit the Prous Science booth, number 26.

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## OTHER USEFUL INFORMATION

**Dates and Venue**

From Sunday, September 1 to Thursday, September 5, 2002

Palau de Congressos de Barcelona  
Avinguda de la Reina Maria Cristina, s/n  
Barcelona, Spain.  
Tel. 34 93 233 20 00

**Symposium Secretariat**

A secretariat desk will be available at level 1 (main entrance).

Address for further correspondence:

ULTRAMAR EXPRESS

Diputació, 238, 2nd. - 08007 Barcelona, Spain

Tel. 34 93 482 71 40 - Fax: 34 93 482 71 58

E-mail: [17ismc@uex.es](mailto:17ismc@uex.es)

[www.ope-uex.com/17ismc](http://www.ope-uex.com/17ismc)

**Official Language**

The official language of the Symposium will be English. No simultaneous translation will be provided.

**Smoking Areas**

As a courtesy to other participants, smokers are kindly asked to note that level 2 is considered as the only smoking area. A special zone is also available in the lunch area.

**Badges and Security**

It will be compulsory for all participants to wear their personal badge at all times while in the Congress venue and during the Social Events, as it will be the official entrance pass to scientific sessions, Commercial Exhibition and Welcome Cocktail.

All participants will find in their documentation envelope a ticket for the Concert as well as for optional excursions and Gala Dinner if they made a reservation. Please do not forget that it will be mandatory to present them to participate in these activities.

**Climate and Clothing**

In September, the weather in Barcelona is magnificent. It is characterised by daytime temperatures between 20° and 25° C, high humidity and sunny days. Very occasional showers might also take place at this time of the year.

**Taxi Service**

Taxis in Barcelona are easily recognisable by their colours (yellow and black).

A green light on the top of the car indicates that it is available. There is usually a supplement for luggage loaded in the back trunk of the car. A taxi from the airport costs an approximately € 15.

## OTHER USEFUL INFORMATION

**Public Transportation**

Barcelona enjoys an excellent public transport system, served by a network of buses and metropolitan subway. The nearest subway station to Palau de Congressos (Congress venue) is Plaça d'Espanya, (line 3 - green, line 1 - red). The same tickets are valid for the bus and the subway. We recommend you to buy a 10 trip ticket (T10; price: € 5.60).

**Travel Information**

IBERIA, Líneas Aéreas de España is the official carrier for the Symposium. Special fares have been agreed upon for the Symposium participants. Please check at your nearest IBERIA office. The Congress Tour Code given by IBERIA is BT21IB21MPE0004. For any request concerning air tickets, please: contact the Secretariat Desk.

**Currency Exchange**

Money can be changed through banks (normal business hours are from 08:30 o 14:00), hotels and other special change offices displaying a "Cambio/Canvi" sign. Take your passport or identity card with you when changing traveller's cheques.

**Tourist Information**

Tourist information will be inserted in the participants' congress bags. More detailed information on visits, excursions cultural events and restaurants will also be available at the Secretariat Desk during the Congress. The Secretariat Desk will also offer information on cultural events as a service to all participants. Main Tourist Office is located in Plaza Catalunya.

**Phone**

Public phones are available at level 1 and 2 of the Congress Palace. You will need either coins (euros only) or phone cards that can be bought at tobacconist's (Shops with sign "Estanco").

**Commercial Hours**

In Barcelona, commercial hours are variable, with shops usually open from 09:30 to 13:30 and from 04:30 to 20:00 on workdays. Large commercial centres remain open from 10:00 to 22:00 Monday to Saturday.

**Attendance Certificate**

Attendance Certificates will be delivered to all participants in their envelope. Certificates of oral and posters communications will be available on request. Please ask for your certificate at the Secretariat Desk (level 1) on Sunday 1 or Monday 2. You will be able to pick it up from Tuesday 3.

**Internet Information**

The final programme of the 17th International Symposium on Medicinal Chemistry is also available at the following web page: [www.ope-uex.com/17ismc](http://www.ope-uex.com/17ismc)



## OTHER USEFUL INFORMATION

### Registration fees for Industrialists, Academics and Students include:

- Access to all the scientific sessions
- Congress bag
- Documentation
- Abstracts Book
- Welcome Cocktail
- Concert (according to availability)
- Coffee breaks
- Lunches on September 2, 3 and 4

The fees do not include:

- Official Dinner
- Excursions
- Personal Insurance: Participants are advised to make their own arrangements regarding travel insurance and medical assistance during the Congress.

### Registration fees for Accompanying Persons include:

- Welcome Cocktail
- Excursion "Panoramic Barcelona" (Half Day excursion) on 2nd September (according to availabilities)
- Concert

The fees do not include:

- Official Dinner
- Excursions
- Personal Insurance: Participants are advised to make their own arrangements regarding travel insurance and medical assistance during the Congress.

## SOCIAL EVENTS & EXCURSIONS

### CONGRESS ATTENDEES & ACCOMPANYING PERSONS

#### Welcome Cocktail

Sunday, September 1, - 19:45  
Congress Venue - Palau de Congressos de Barcelona

#### Concert at Santa Maria Del Mar (partially sponsored by Chemical Computing Group)

Monday, September 2, - 20:30  
The Basilica of Santa Maria del Mar is a gothic building of extraordinary beauty. It has a remarkable, spacious interior structure and rose window, dating from the mid-15th century

### ACCOMPANYING PERSONS

#### Monday, September 2 - Barcelona City Tour

After visiting the Gothic Quarter and the Olympic Port, this tour will bring you to the Montjuïc Mountain. You will enjoy the fantastic panoramic view of the city and be able to discover the installations of the Olympic Ring as well as the "Pueblo Español".

### OPTIONAL SOCIAL EVENTS

#### Gala Dinner

Wednesday, September 4  
Hotel Fira Palace  
Price: € 75

### OPTIONAL EXCURSIONS

#### Tuesday, September 3 - Girona -Figueras & Dalí Museum

This tour will allow you discovering the historical city of Girona, specially its cathedral and Jewish Quarter. Continuation onto Figueras where you will have lunch and discover the Dalí Museum

From 08:30 to 18:30 hrs. (Lunch Included)

Price: € 82

#### Wednesday, September 4 - Montserrat

Visit to the holy mountain with its impressive rock formations and the Royal Basilica where we can see the Black Virgin. Singing session by the famous "Escolania" choir.

From 09:30 to 14:30 hrs. (without lunch).

Price: € 39

#### Wednesday, September 4 - Modernism & Museo Picasso

This tour includes a panoramic view of Casa Batlló, Casa Milà, Sagrada Família, Monumental Bull Ring as well as a visit to the "Parc Güell" (also by Gaudí). The second part of the tour will be dedicated to the visit of the Picasso Museum.

From 15:30 to 18:30 hrs. (without lunch)

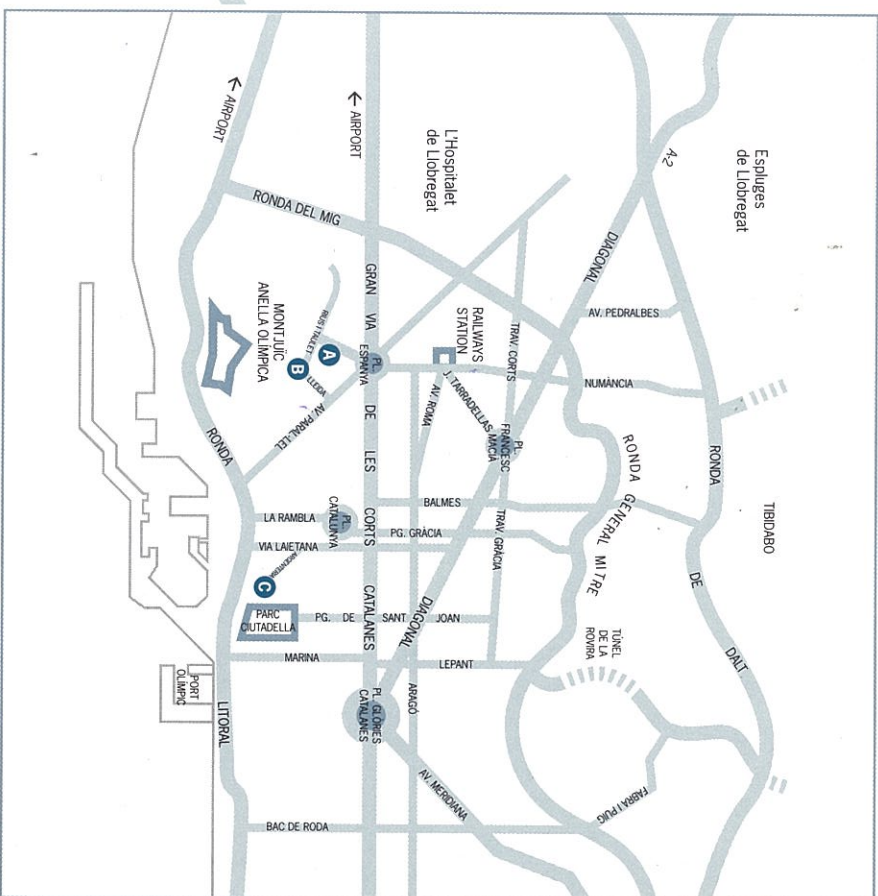
Price: € 32

Tickets can be bought at the Secretariat Desk.

A minimum of 25 participants is required for the excursions to go ahead.



## SYMPOSIUM VENUES



- A: Congress Venue  
 B: Hotel Fira Palace  
 (Gala Dinner venue)  
 C: Santa Maria del Mar  
 (Concert venue)

molecular operating environment

# MOE



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