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# Joint Meeting on Medicinal Chemistry

## Vienna, Austria
## June 20-23, 2005


Organized by the Austrian Chemical Society,
Medicinal Chemistry Section, the Austrian Pharmaceutical Society
and the Department of Medicinal/Pharmaceutical Chemistry.

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EFMC

# WELCOME

The Organizing Committee cordially invites you to the **Austrian-German-Hungarian-Italian-Polish-Spanish Joint Meeting on Medicinal Chemistry (JMMC)** to be held in Vienna, Austria during the period June 20 - 23, 2005 under the auspices of the European Federation for Medicinal Chemistry.

The Vienna meeting will continue a tradition established at the three previous Joint Meetings of the series, held in Taormina (Italy) in 1999, Budapest (Hungary) in 2001 and Krakow (Poland) in 2003.

Following the spirit of the previous meetings we envision a stimulating scientific event where scientists meet in one plenum to present & discuss all aspects of medicinal chemistry. There will be 5 plenary lectures, 20 key lecturers, 11 oral short communications and two poster sessions with more than 200 posters on display.

The Vienna Symposium will focus on the following topics:

- Lead & Drug likeness
- Chemogenomics, Combichem & other developing fields in Medicinal Chemistry
- Medicinal Chemistry Case studies & Natural Product Synthesis
- Oncology
- Alzheimer and Central Nervous System disorders
- Computer aided molecular design & virtual screening

Vienna, right in the center of the European Union, with its commitment to research, its prospering economy and its rich cultural life, stimulating arts and music scene is the perfect city to combine science and tourism.

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Chairman

Gerhard Ecker
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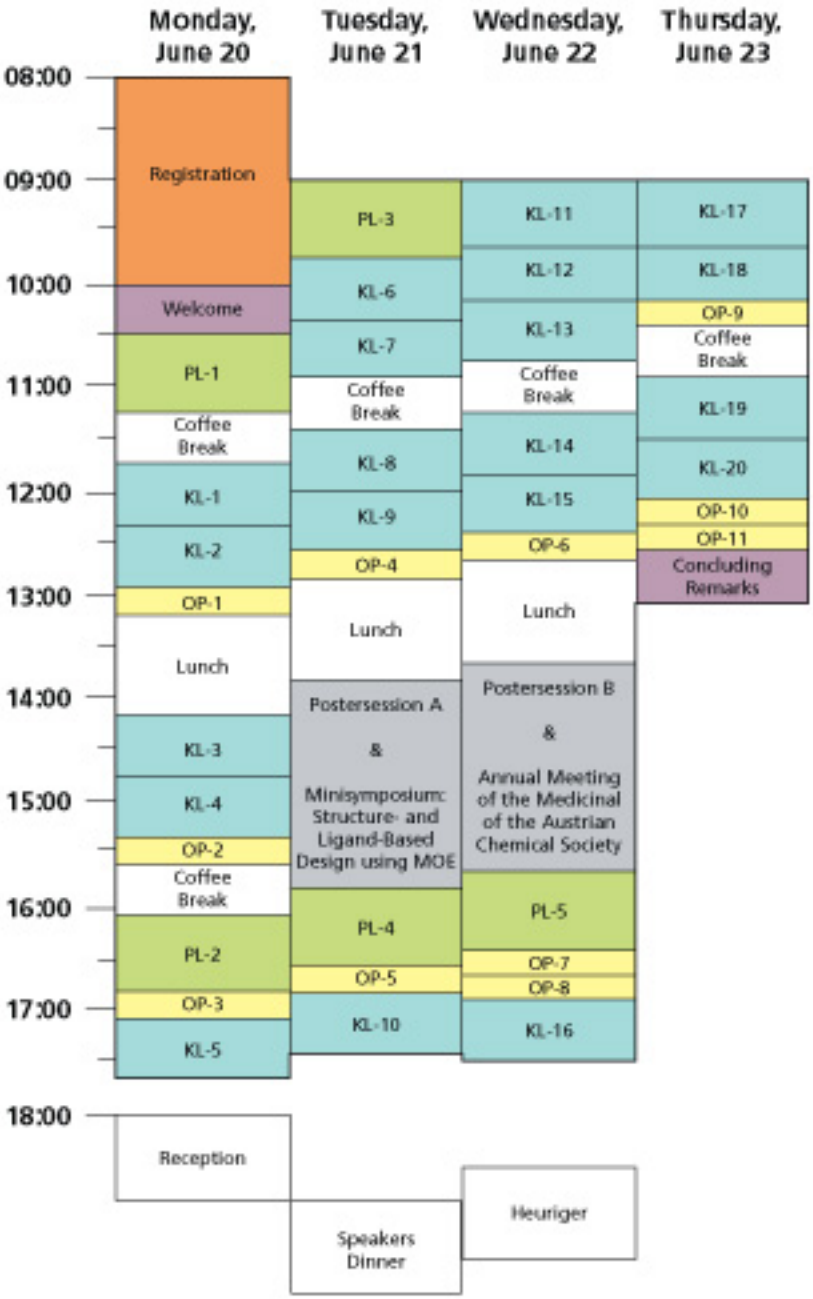
# TIME TABLE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Tuesday, June 21
Wednesday, June 22
Thursday, June 23
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11:00
12:00
13:00
14:00
15:00
16:00
17:00
18:00
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Coffee Break
KL-1
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OP-1
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KL-3
KL-4
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PL-2
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PL-3
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KL-7
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KL-8
KL-9
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OP-9
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KL-20
OP-10
OP-11
Concluding Remarks
Reception
Speakers Dinner
Heuriger

# KEY INFORMATION for all attendees

**Conference Venue:** University of Vienna
Dr. Karl Lueger Ring 1, 1010 Vienna, banqueting hall

**Conference Language:** English

**Registration and Information Desk** will be located at the entrance to the banqueting hall. Registration starts on Monday, June 20, 8:00 to 18:00 and will be open Tuesday to Wednesday from 8:45 to 18:00 and Thursday 8:45 to 12:00. Please note that because the symposium is fully booked no onsite-registration will be available.

**Badges** will be handed out to every participant. It will be compulsory for all participants to wear the badges while at the conference venue. For identification purpose the following color scheme applies:

Participants (white), Accompanying persons (red), Lecturers (green), Chairpersons & Organizers (purple), Exhibitors (blue)

**General Information**

- A buffet lunch will be served every day (see time table) in the hallways outside the banqueting hall (included in registration fee for participants)
- Please do not miss to visit the Commercial Exhibition in the small banqueting hall.
- Coffee breaks will be served in the Commercial Exhibition Area (small banqueting hall, see time table)
- On Monday, June 20th, all participants and their accompanying persons are cordially invited to the Welcome Reception starting at 18:00 at the symposium venue
- On Wednesday, June 22nd, all participants that signed up for the "Heurigen" are cordially invited to the Augustinerkeller.
  Adress: Augustinerstraße 1, 1010 Wien starting at 18:30.

# KEY INFORMATION Scientific presentations

**If you are a session chairperson**, you are kindly asked to be in the banqueting hall 15´prior to the beginning of the session to meet with the speakers. There are three speech formats:

- 45´plenary lectures; 35´ key lectures and 15´oral communications. All formats include already discussion time and the chairpersons are earnestly asked to strictly follow the scheduled times.

**If you are a speaker**, you are kindly asked to be in the banqueting hall 15´prior to the beginning of the session to meet with the chairpersons and the technician in charge of the projection.

The conference lecture hall will be equipped only with a video beamer (resolution 1024 x 768; standard XGA). The lecture hall cannot be completely darkened! Please prepare your slides for maximum contrast.

The standard format for presentations is MS-PowerPoint (95,97, 2000, 2003). Please use the "embedded fonts" to avoid certain problems when projecting files prepared on a different computer. For all other types of video presentation an own laptop must be used. Authors can carry their presentation on a CD-Rom or on an USB stick. Files must be loaded onto the presentation laptop before the start of the session! Thus, speakers have to visit the information desk before their presentation. A preview of the presentations will be at the information desk and during the breaks in the banqueting hall

**If you present a poster**, please see the alphabetically ordered list of posters in this program for the code and the session assigned to your poster. Each poster has be scheduled in one of the two poster sessions

**Session A**, Tuesday, June 21, 13:50 - 15:50 (from PO1 to PO100)

**Session B**, Wednesday, June 22, 13:40 – 15:40 (from PO101 to PO204)

The poster boards will be numbered according to the program. Authors are requested to be in front of their poster during the official session time and remove their posters at the end of the session.

# SCIENTIFIC PROGRAMME

## Monday, 20.06.2005

| | |
|---|---|
| 10:00 - 10:30 | Inauguration |
| 10:30 - 11:15 | **PL1 Herbert Waldmann** (D)<br>Protein Structure Similarity Clustering (PSSC) and Natural Product Structure as Guiding Principle for Chemical Genomics |
| 11:15 - 11:45 | Coffee |
| **Session 1** | **Chair: Hugo Kubinyi, Maria-José Camarasa** |
| 11:45 - 12:20 | **KL1 Jordi Mestres** (E)<br>Computational Chemogenomics: Extracting Knowledge from Biochemical Data |
| 12:20 - 12:55 | **KL2 John Tallarico** (US)<br>Finding Protein Targets for Drugs - The Chemogenetic Approach |
| 12:55 - 13:10 | **OP1 Hans-Dieter Junker** (D)<br>Chemical Microarrays,- Tools for High Throughput Fragment-based Drug Discovery |
| 13:10 - 14:10 | Lunch |
| **Session 2** | **Chair: Peter Ettmayer, Zdzislaw Chilmonczyk** |
| 14:10 - 14:45 | **KL3 Giuseppe A.M. Giardina** (I)<br>Microwave-Assisted Highthroughput Chemistry in Lead Generation and Optimization |
| 14:45 - 15:20 | **KL4 Wolfgang Binder** (A)<br>Lipid Rafts and their Biological Significance |
| 15:20 - 15.35 | **OP2 Jaroslav Skubak** (A)<br>Microwave Assisted and Conventional Mono Aryl Substitution of Diazabicycloalkanes by Encapsulated Palladium Coupling |
| 15:35 - 16:05 | Coffee |
| **Session 3** | **Chair: Oliver Kappe, Gerd Schnorrenberg** |
| 16:05 - 16:50 | **PL2 Ulrich Stilz** (D)<br>Strategies for Lead Finding and Lead Optimization Utilizing Experimental and Computational Approaches |
| 16:50 - 17:05 | **OP3 Pawel Wiczling** (PL)<br>Application of Simultaneous pH and Organic Solvent Gradient RP HPLC in Determination of Pharmacokinetics-affecting Parameters of Drugs |
| 17:05 - 17:40 | **KL5 Ferenc Hudecz** (H) Drug Targeting by Peptide Conjugates |
| 18:00 | Welcome Reception, conference venue |

# SCIENTIFIC PROGRAMME

**Tuesday, 21.06.2005**

| | |
|---|---|
| **Session 4** | **Chair: Gerhard Ecker, Katarzyna Kiec-Kononowicz** |
| 09:00 - 09:45 | **PL3 Tudor I. Oprea** (US)<br>Pursuing Leadlikeness in Pharmaceutical Research |
| 09:45 - 10:20 | **KL6 György Dormán** (H)<br>In Silico Approaches Generating Novel Compound Series in Lead Optimization |
| 10:20 - 10:55 | **KL7 Jaroslaw Polanski** (PL)<br>Modeling Robust QSAR |
| 10:55 - 11:25 | Coffee |
| **Session 5** | **Chair: Péter Mátyus, Guiseppe Ronsisvalle** |
| 11:25 - 12:00 | **KL8 Slawomir Filipek** (PL)<br>Functional Oligomers of Rhodopsin - a G Protein-Coupled Receptor Template |
| 12:00 - 12:35 | **KL9 Federico Gago** (E)<br>In Silico Medicinal Chemistry and Pharmacology of Natural Products: Understanding Biological Effects Through Molecular Modeling and Molecular Dynamics Simulations |
| 12:35 - 12:50 | **OP4 Krzysztof Jozwiak** (PL)<br>Multidisciplinary Characterization of Molecular Interactions between Nicotinic Acetylcholine Receptors and its Ligands |
| 12:50 - 13:50 | Lunch |
| 13:50 - 15:50 | Poster A & Minisymposium: Structure - and Ligand Based Design using MOE |
| **Session 6** | **Chair: Ulrich Stilz, Roberto Pellicciari** |
| 15:50 - 16:35 | **PL4 Hugo Kubinyi** (D)<br>From Leads to Drugs |
| 16:35 - 16:50 | **OP5 Dirk Classen-Houben** (A)<br>3D-QSAR and Virtual Screening of Protein-Tyrosine-Phosohatase 1B Inhibitors |
| 16:50 - 17:25 | **KL10 Carlo Melchiorre** (I)<br>Discovery of Multipotent Drugs for the Treatment of Alzheimer's Disease |
| 19:30 | Speakers dinner, Sky Restaurant |

# SCIENTIFIC PROGRAMME

**Wednesday, 22.06.2005**

| | |
|---|---|
| **Session 7** | **Chair: Christian Noe, Janina Karolak-Wojciechowska** |
| 09:00 - 09:35 | **KL11 László Harsing** (H)<br>2,3-Benzodiazepines: Multiple Pharmacological Actions and Structure-Activity Relationship |
| 09:35 - 10:10 | **KL12 Barbara Nawrot** (PL)<br>Use of Small Inhibitory Nucleic Acids for Down-Regulation of Genes Involved in Alzheimer's Disease |
| 10:10 - 10:45 | **KL13 Maria L. López-Rodriguez** (E)<br>The Endogenous Cannabinoid System: From the Molecules to the Therapeutic Applications |
| 10:45 - 11:15 | Coffee |
| **Session 8** | **Chair: Eric Haaksma, Isabel Fernandez** |
| 11:15 - 11:50 | **KL14 Andreas Schoop** (A)<br>Inhibition of the Cell Cycle Kinase CDK1 by 2,4-Diamino-Pyrimidines |
| 11:50 - 12:25 | **KL15 Kálmán Hideg** (H) New PARP inhibitors |
| 12:25 - 12:40 | **OP6 Sonsoles Martin-Santamaria** (E)<br>Adrenomedullin: A New Target for the Design and Synthesis of Drugs |
| 12:40 - 13:40 | Lunch |
| 13:40 - 15:40 | Poster B & Annual Meeting of the Medicinal Chemistry Section of the Austrian Chemical Society |
| **Session 9** | **Chair: Ferran Sanz, Roman Kaliszan** |
| 15:40 - 16:25 | **PL5 Angelo Carotti** (I)<br>In Silico Design and Focused Solid Phase Synthesis of New, Selective Enzyme Inhibitors with Potential in Cancer and Neurological Therapies |
| 16:25 - 16:40 | **OP7 Antonio Lavecchia** (I)<br>Novel Highly Potent Adenosine Deaminase Inhibitors Containing the Pyrazolo[3,4-d]pyrimidine Ring System. Synthesis, Structure-activity Relationships and Molecular Modeling Studies |
| 16:40 - 16:55 | **OP8 Máté Bubenyák** (H)<br>Synthesis of Pentacyclic Alkaloid Hybrides |
| 16:55 - 17:30 | **KL16 Mario Varasi** (I)<br>3-Amino-1H-pyrazole Derivatives as Useful Scaffolds for the Generation of New Kinase Inhibitors |
| 18:30 | Heuriger, Augustinerkeller, Augustinerstraße 1, 1010 Wien |

# SCIENTIFIC PROGRAMME

**Thursday, 23.06.2005**

| | |
|---|---|
| **Session 10** | **Chair: Tudor I. Oprea, Janos Wölfling** |
| 09:00 - 09:35 | **KL17 Johann Mulzer** (A)<br>Progress in the Total Synthesis of Polycyclic Natural Products |
| 09:35 - 10:10 | **KL18 Peter Nussbaumer** (A)<br>Inhibition of Steroid Sulfatase: a New Approach to Treat Estrogen- and Androgen-Dependent Diseases |
| 10:10 - 10:25 | **OP9 Iana Vazzana** (I)<br>Novel Quinolizidinyl Derivatives as Antiarrhythmic Agents |
| 10:25 - 10:55 | Coffee |
| **Session 11** | **Chair: Gerhard Ecker, Peter Ettmayer** |
| 10:55 - 11:30 | **KL19 Barbara Malawska** (PL)<br>New Development in alfa-1 Adrenergic Receptors Antagonists |
| 11:30 - 12:05 | **KL20 Michael Bös** (CA)<br>The Identification of HCV Polymerase Inhibitors: A Showcase of Modern Drug Discovery |
| 12:05 - 12:20 | **OP10 Marcello Leopoldo** (I)<br>N-(1,2,3,4-tetrahydronaphthalen-1-yl)-4-Aryl-1-piperazinealkylamides as 5-HT7 Receptor Agents |
| 12:20 - 12:35 | **OP11 Michael Graupe** (US)<br>Structure Based Design of Cathepsin S Inhibitors |
| 12:35 - 12:50 | Concluding Remarks |

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# COMMERCIAL EXHIBITIONS

The exhibitions can be visited in the small banqueting hall from Monday to Wednesday from 10:00 to 18:00.

The new **ABCR** Fluorochemicals catalogue 2005 is available at the Vienna Medicinal Chemistry meeting, featuring over 8000 partially unique building blocks. Please also use the new sub-structure search at www.abcr.de. Take/order your free copy of either the new Fluorochemicals catalogue, or any other of our various speciality catalogues on Organic, Inorganic, Metal-Organic, Biochemical, Catalytical or Silicon chemistry. Competent assistance by our chemists, reliable worldwide deliveries at fair prices and excellent quality have made ABCR "preferred supplier" of many pharmaceutical customers.

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# OPTIONAL TOURS

Austropa Interconvention offers all participants excursions to discover Vienna and the surrounding area.

**Viennese Woods**

Tuesday 21.06.05 Departure 14:45 € 42.00 per person

**City tour including Schönbrunn**

Wednesday, 22.06.05 Departure 09:45 € 34.00 per person

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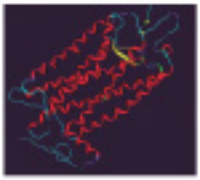

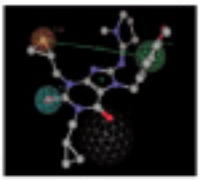

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