Final Programme

XVIIIth

International Symposium on Medicinal Chemistry

Copenhagen, Denmark & Malmoe, Sweden
August 15-19, 2004

WELCOME

Dear Colleagues,

On behalf of the Organizing Committee, I sincerely wish to welcome you to the XVIIIth International Symposium on Medicinal Chemistry (ISMC 2004), to be held in Copenhagen and Malmö during the period August 15 – 19, 2004.

The ISMC Symposia, held under the umbrella of the European Federation of Medicinal Chemistry (EFMC), are major scientific events in the fields of medicinal chemistry and drug design. Multi- and interdisciplinarity are fundamental characteristics of these research areas. With the growing number of disciplines in the field of medicinal chemistry, optimal integration of scientific disciplines is a constantly growing challenge to medicinal chemists. I do hope that ISMC 2004 will form a forum for intense discussions of these aspects, and that new lines and models for the further development of medicinal chemistry as a science may emerge from these interactions.

Most of the ISMC 2004 scientific events are organized in Copenhagen, but the Wednesday arrangements will take place in Malmoe. This structure of the Symposium will allow the participants to visit the Danish as well as the Swedish side of Medicon Valley covering Copenhagen and Malmoe/Lund in Sweden.

Medicon Valley is a fast-growing pharmaceutical biotech region, and it is expected that the broad spectrum of Medicon Valley pharmaceutical scientists and the ISMC 2004 participants will experience mutually stimulating scientific interaction during the symposium. I do hope that the many cultural and tourist attractions of the Medicon Valley cities may form exciting frames for the interactions.

Welcome to the ISMC 2004

Povl Krogsgaard-Larsen, Chairman

COMMITTEES

Scientific Advisory Committee

Paul S. Anderson	(USA)	Rob Leurs	(The Netherlands)
Peter Andrews	(Australia)	Kristina Luthman	(Sweden)
Lars-Erik Arvidsson	(Sweden)	John McCall	(USA)
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Klaus Bøgesø	(Denmark)	Peter Nielsen	(Denmark)
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Peter Ettmayer	(Austria)	Roberto Pellicciari	(Italy)
Wolfgang Froestl	(Switzerland)	Ferran Sanz	(Spain)
Robin Ganellin	(UK)	Richard Silverman	(USA)
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Rolf Hartmann	(Germany)	Camille Wermuth	(France)
Jan Kihlberg	(Sweden)	Patrick Woster	(USA)
Toshi Kobayashi	(Japan)		

Organizing Committee

Chairman: Povl Krogsgaard-Larsen, Denmark

Anette Birck	Denmark, Sweden	Rolf Johansson	Sweden
Hans Bräuner-Osborne	Denmark	Anders Karlén	Sweden
Klaus Gundertofte	Denmark	Tommy Liljefors	Denmark
Uli Hacksell	USA	Henk Timmerman	The Netherlands
Märit Johansson	Sweden		

EFMC
European Federation for Medicinal Chemistry

Danish Society for Pharmacology and Toxicology

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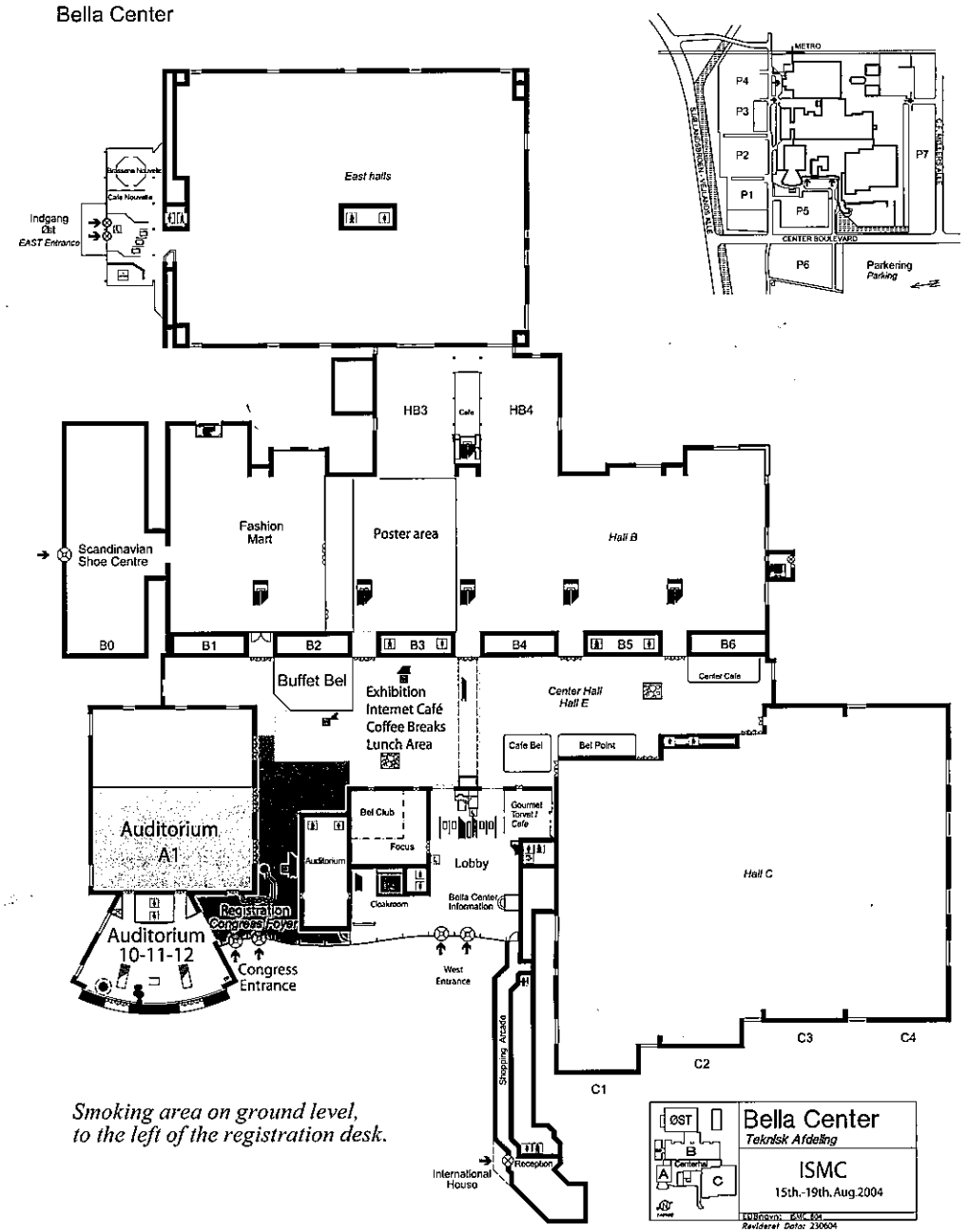
CONTENTS

CONGRESS VENUE



Smoking area on ground level,
to the left of the registration desk.

- The Symposium is divided into four parallel sessions.
  For Auditorium see the scientific programme.
  (Please see enclosed map of the Venue).

- On Sunday, August 15, after the Opening Lecture, a Welcome Reception will be served to all attendants, and their accompanying persons in the Exhibition area.

- Posters will be displayed during the whole Symposium time but will only be manned during one of the sessions. On Monday all posters with odd numbers will be manned and on Tuesday all posters with even numbers will be manned. During the postersesion on Thursday manning is optional.
  (See Scientific programme and poster lists in the abtracts book.)

- A large Exhibition can also be visited.

- There will be free access to Internet at the Internet Café located in the exhibition area.

- A lunchbox will be served every day in the Exhibition area. A ticket for each lunch you will find in your envelope in the Congress bag. You can have your lunch seated at or walk around in the Exhibition or poster area.

- Coffee breaks will be served in the Exhibition area every day, please see the programme.

- Some lectures will be video recorded and made available through Internet from Sunday, August 22 at the following addresses:

  www.prous.com/ismc2004
  www.ismc2004.dk
  www.ismc2004.dk/webcasts

KEY INFORMATION FOR ALL ATTENDANTS

If you are 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 sessions to meet with speakers.

There are three speech formats:
- 45' lectures devided into 40' presentation and 5' discussion
- 30' lectures devided into 25' presentation and 5' discussion
- 15' oral communications

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.

A preview room for presentations is available during the Symposium. It is located on Bella Center, room 4 on 1st floor, and will be open throughout the Symposium.

For any request, please feel free to contact the organisation staff at the Secretariat Desk located at the main entrance.

If you present a poster...

The posterboards will be 243 cm (height) by 97 cm (width), which corresponds to 95 by 38 inches. Posters are best put up with poster pads or tape.

The poster should be mounted Monday morning August 16, 2004 and dismounted Thursday August 19, 2004 after the afternoon poster session.

All posters will be shown at all three sessions, but will only be manned during one of the sessions. On Monday, August 16 all posters with odd numbers will be manned during the poster session. On Tuesday, August 17 all posters with even numbers will be manned. During the poster session on Thursday manning is optional. For posters without numbers manning is optional.

Please see the alphabetically ordered list of posters in the abstract book to find what poster board number that is allotted your poster. If your poster does not have any number please place your poster among poster boards that do not have any numbers given.

Dates and Venue
The Symposium takes place at the Bella Center from Sunday, August 15 to Thursday, August 19, 2004.
Venue address:
Bella Center
Center Boulevard 5
DK-2300 Copenhagen S, Denmark

On Wednesday, August 18, the Symposium takes place at Slagthuset, Malmoe, Sweden.
Venue address:
Slagthuset
Jörgen Kocksgata 7A
211 20 Malmoe, Sweden

Symposium Secretariat
A secretariat desk will be available at the main entrance.
Telephone: +45 32622531
Fax: +45 32622520

Registration/Hospitality desk-opening hours during the Symposium:

Sunday, August 15	hrs. 16.00-20.00
Monday, August 16	hrs. 08.00-18.00
Tuesday, August 17	hrs. 08.00.18.00
Thursday, August 19	hrs. 08.30-16.00

After the Symposium:
ISMC 2004-06-24 c/o DIS Congress Service A/S
Herley Ringvej 2C
DK-2730 Herlev, Denmark
Telephone: +45 4492 4492
Telefax: +45 4492 5050

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 asked to note that the Auditorium Foyer to the left of the registration desk is considered as the only smoking area.

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

All participants will find in their documentation envelope lunch tickets as well as tickets for optional excursions 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
The weather in Denmark in August is normally very pleasant, usually sunny. However, on occasion an umbrella may be useful. Daytime average temperature is around 22° C, evening Temperature around 15° C

Local transportation
From the city centre the metro takes you to the Metrostration Bella Center.

Registration fees for Industrialists, Academics and Students include:
- Access to all the scientific sessions
- Congress bag
- Final Programme Book
- Abstracts Book
- Welcome Reception
- Coffee/tea during the breaks on Symposium days
- Lunches on August 16, 17, 18 and 19
- Transportation Copenhagen-Malmoe on Wednesday, August 19, and participation in the Get Together in Malmoe, Sweden

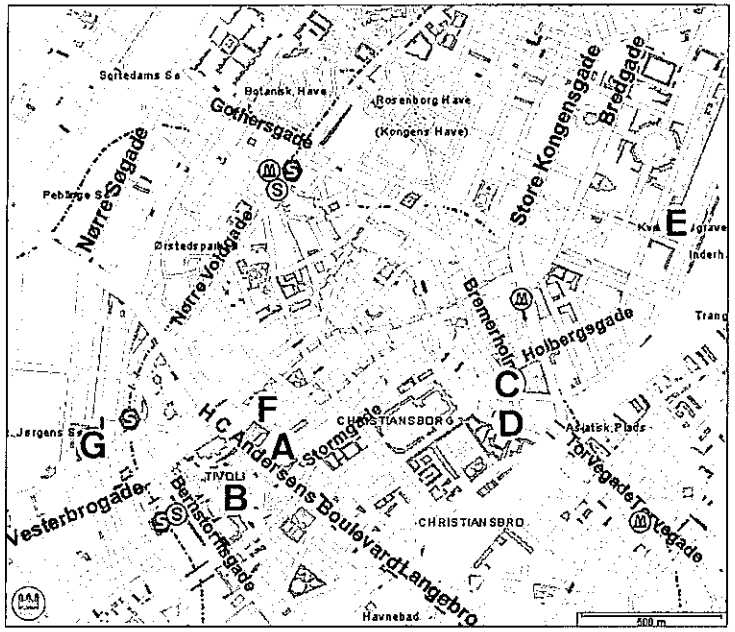
Registration fees for Accompanying Persons include:
- Welcome Reception
- Transportation Copenhagen-Malmoe on Wednesday, August 19, and participation in the Get Together in Malmoe, Sweden

The fees do not include:
- Concert on Monday, August 16
- Excursions
- Personal insurance: Participants are advised to make their own arrangements regarding travel insurance and medicinal assistans during the Symposium.

The day in Malmoe, Wednesday 18
Buses will pick you up for Malmoe 8:45 at the stops indicated on the map enclosed. Trains will take you back to Copenhagen every 20 minutes from Malmoe Central station (map will be distributed on site). Please note that after 01:00 hrs you have to pay an extra fee and there is only one train every hour.

MAPS

Copenhagen



Landmarks:

A: City Hall
B: The Tivoli Gardens
C: Holmens Church*
D: Børsen "the Old Stock Exchange*

*Concert and Reception on Monday, August 16 – purchased ticket is required for this event.

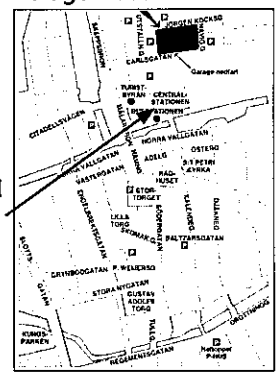
Bus departure for Malmö on Wednesday, August 18 – Designated pick-up places:

E: In front of Hotel Sofie Amalie, Sankt Annæ Plads 21
F: In front of Hotel Palace (next to City Hall), Rådhuspladsen 57
G: In rear of the Hotel Copenhagen Scandic Hotel, Nyrupsgade

Please note that the last bus departs at 08:45 hrs.

Malmoe

Slagthuset



SCIENTIFIC PROGRAMME

The scientific programme consist of a mixture of plenary lectures, four parallel lecture sessions and poster sessions.
Plenary lectures (except Wednesday) and session with the letter A will be held in Auditorium A1, whereas sessions with the letter B, C and D will be held in Auditorium 10, 11 and 12, respectively.

	Starting time
SUNDAY	
Opening ceremony and welcome *Povl Krogsgaard-Larsen, Chairman* Danish University of Pharmaceutical Sciences, Copenhagen, Denmark	17:40
Award ceremony *Ferran Sanz*, EFMC Chairman, Universitat Pompeu Fabra, Barcelona, Spain	
Inaugural Lecture: *Paul Anderson*, Lansdale, PA, USA Medicinal chemistry – An evolving structure-driven science	18:45
Welcome Reception	19:30
MONDAY	
Prous Award Lecture: *Oliver Kappe*, Karl-Franzens-Universität, Graz, Austria High-speed microwave synthesis: enabling technology for organic, medicinal and chemistry combinatorial Chairman: *Ferran Sanz*	9:00
Exhibition and coffee	9:45
Dementia & memory / **Natural toxins as leads** / **Cancer new targets** / **Drug discovery new strategies**	10:30
Poster session (posters with odd numbers) - Lunch	12:30
Enzymes I proteases structure & inhibitors / **Pain new targets** / **Advances in cardiovascular therapy** / **Chemical diversity and library design**	14:30
Coffee	15:45
Enzymes II kinases structure & inhibitors / **CNS I psychosis** / **Nucleic acid therapeutics** / **Receptors I GPCRs structure & ligands**	16:15 (17:30 End)

Programme for parallel lecture sessions:

Session 1A Dementia & memory
Chairman: *Wolfgang Froestl*, Novartis Pharma, Basel, Switzerland
Key lectures:
- *Gregory M. Rose*, Memory Pharmaceuticals, Montvale, NJ, USA: Developing treatments for age-related memory loss (10:30-11:15)
- *Brian P. Lockhart*, Servier, Croissy-sur-Seine, France: Cognitive enhancing or neuroprotective drugs for the treatment of dementia, why? when? which? (11:15-12:00)

Oral presentations:
- *Ramin Faghih*, Abbott Laboratories, IL, USA: [3H]-A-349821: a novel non-imidazole histamine H3 receptor radioligand (12:00-12:15)
- *Christopher Johnson*, GSK, Harlow, UK: The discovery of selective brain penetrant 5-HT6 receptor antagonists (12:15-12:30)

Session 1B Natural toxins as leads
Chairman: *Kristian Strømgaard*, The Danish University of Pharmaceutical Sciences, Copenhagen, Denmark
Key lectures:
- *André Ménez*, CEA, Gif-sur-Yvette, France: From toxins to drugs (10:30-11:15)
- *Baldomero M. Olivera*, University of Utah, Salt Lake City, UT, USA: The venomous cone snails: 50 million years of drug development and medicinal chemistry (11:15-12:00)

Oral presentations:
- *Elizabeth M. Doherty*, Amgen, Thousand Oaks, CA, USA: Discovery of Potent Antagonists of the TRPV1 Channel. Structure-Activity Relationship of N-Aryl Cinnamides (12:00-12:15)
- *Søren Brøgger Christensen*, The Danish University of Pharmaceutical Sciences, Copenhagen, Denmark: Targeting of Thapsigargin: A New Concept for Treatment of Slowly Developing Cancer Diseases (12:15-12:30)

Session 1C Cancer: new targets
Chairman: *Fredrik Björkling*, LEO Pharma, Ballerup, Denmark
Key lectures:
- *Paul W. Manley*, Novartis, Basel, Switzerland: Anthranilic acid derivatives: VEGF-R kinase inhibitors for anti-angiogenic therapy in cancer (10:30-11:15)
- *Steven Elmore*, Abbott Laboratories, Abott Park, IL, USA: Targeting apotosis for cancer therapy: Discovery of small molecule inhibitors of anti-apoptotic Bcl-2 family proteins (11:15-12:00)

Oral presentations:
- *Sook Wah Yee*, Cardiff University, Cardiff, UK: Design and synthesis of P450 enzymes inhibitors as differentiating agent for androgen-independent prostate cancer (12:00-12:15)
- *Antonello Mai*, Università degli Studi di Roma, Rome, Italy: Design, synthesis, and biological evaluation of uracil-based hydroxy-amides (UBHAs) as a new class of HDAC inhibitors (12:15-12:30)

Session 1D Drug discovery: new strategies
Chairman: *Ferran Sanz*, IMIM - Universitat Pompeu Fabra, Barcelona, Spain
Key lectures:
- *Graham W. Richards*, Oxford University, Oxford, UK: Pattern recognition and grid computing in drug discovery (10:30-11:15)
- *James Fickett*, AstraZeneca, Waltham, MA, USA: Systems biology and drug discovery (11:15-12:00)

Oral presentations:
- *Gerhard Ecker*, University of Vienna, Vienna, Austria: An atomic detail model of the bacterial ABC-transporter LmrA from Lactococcus Lactis (12:00-12:15)
- *Thierry Langer*, University of Innsbruck, Innsbruck, Austria: Mining pharmacophoric content from protein-ligand-complex information as a basis for activity profiling (12:15-12:30)

Session 2A Enzymes I: proteases - structure & inhibitors
Chairman: *Anders Hallberg*, Uppsala University, Uppsala, Sweden
Key lecture:
- *Montse Llinás-Brunet*, Boehringer-Ingelheim, Quebec, Canada: The discovery of BILN 2061, an NS3 protease inhibitor with antiviral effects in humans infected with hepatitis C virus (14:30-15:15)

Oral presentations:
- *Jeffrey A. Robl*, Bristol-Myers Squibb, Princeton, NJ, USA: Design, synthesis, and pharmacology of BMS-477118: A long-acting, orally active dipeptidyl peptidase IV inhibitor for the treatment of yype II diabetes (15:15-15:30)
- *Jian Jeffrey Chen*, Roche Bioscience, Palo Alto, CA, USA: Discovery and synthesis of orally active dual TNF / MMP inhibitors as anti-rhematoid arthritis drugs (15:30-15:45)

Session 2B Pain: new targets
Chairman: *Lars Terenius*, Karolinska sjukhuset, Stockholm, Sweden
Key lecture: *Mirek Tomaszewski*, AstraZeneca R&D, Montréal, Canada: Discovery of pain targets - GPCR target class approach (14:30-15:15)
Oral presentations:
- *Ronald Palin*, Organon Laboratories, Newhouse, UK: Opioid Receptor Like (ORL-1) agonists as novel analgesics (15:15-15:30)
- *Daniela Fattori*, Menarini Ricerche, Pomezia, Italy: Solid phase synthesis using the "Fragment Approach": Generation of a new class of NK2 receptor antagonists (15:30-15:45)

Session 2C Advances in cardiovascular therapy (ACS session)
Chairman: *Patrick Woster*, Wayne State University, Detroit, MI, USA
Key lecture:
- *Robert J. Linhardt*, Rensselaer Polytechnic Institute, Troy, NY, USA: Heparin and related molecules as multi-pharmacological agents (14:30-15:15)

Oral presentations:
- *Samuel Chackalamannil*, Schering-Plough Research Institute, Kenilworth, NJ, USA: Discovery of potent himbacine-based thrombin receptor antagonists (15:15-15:30)
- *Prabhakar K. Jadhav*, Indianapolis, IN, USA: Discovery of potent, orally bioavailable non-steroidal mineralocorticoid receptor antagonist (15:30-15:45)

Session 2D Chemical diversity and library design
Chairman: *Paul Leeson*, AstraZeneca, Leicestershire, UK
Key lecture:
- *Mark Gardner*, Pfizer Central Research, Sandwich, Kent, UK: Library design and follow-up - does more hits mean more drugs? (14:30-15:15)

Oral presentations:
- *Roger Crossley*, BioFocus Discovery, Saffron Walden, Essex, UK: Increase in project efficiencies gained by the use of focused libraries (15:15-15:30)
- *Tim J. Cheeseright*, Cresset BioMolecular Discovery, Letchworth , UK: New leads for GPCR projects: A real breakthrough in virtual screening (15:30-15:45)

Session 3A Enzymes II: kinases - structure & inhibitors
Chairman: *Joe Shih*, Eli Lilly, Indianapolis, IN, USA
Key lecture:
- *John Regan* , Boehringer Ingelheim, Ridgefield, CT, USA: The structural, kinetic and anti-inflammatory properties of BIRB 796, an inhibitor of p38 MAP kinase (16:15-17:00)

Oral presentations:
- *Birgit Masjost*, Roche Diagnostics, Penzberg, Germany: Structure-based optimization of novel azepane derivatives as PKB inhibitors (17:00-17:15)
- *Thomas A. Engler*, Lilly Research Laboratories, Indianapolis, IN, USA: The effects of highly selective and potent inhibitors of GSK3 on the insulin and Wnt signaling pathways (17:15-17:30)

Session 3B CNS I: psychosis
Chairman: *David Weiner*, ACADIA Pharmaceuticals, San Diego, CA, USA
Key lecture:
- *Carol A Tamminga*, University of Texas Southwestern Medical Center, Dallas, TX, USA: Schizophrenia: What we know and what we need to know (16:15-17:00)

Oral presentations:
- *Timo Heinrich*, Merck KGaA, Darmstadt, Germany: Novel substituted indoles as highly selective 5-HT2A antagonists (17:00-17:15)
- *Ulrike Holzgrabe*, University of Würzburg, Würzburg, Germany: Systematic development of enhancers of ligand binding to muscarinic acetylcholine receptors: bis(ammonio)alkane-type compounds (17:15-17:30)

Session 3C Nucleic acid therapeutics
Chairman: *Peter E. Nielsen*, University of Copenhagen, Copenhagen, Denmark
Key lectures:
- *Frank Bennett*, Isis Pharmaceuticals, Carlsbad, CA, USA: Progress in antisense oligonucleotide based therapeutics and issues for the future (16:15-17:00)
- *Eugen Uhlmann*, Coley Pharmaceutiacl, Langenfeld, Germany: Recent studies to the mechanisms and application of Immune stimulatory CgG TLR9 agonists (17:00-17:45)

Session 3D Receptors I: GPCRs - structure & ligands
Chairman: *Rob Leurs*, Vrije Universiteit, Amsterdam, The Netherlands
Key lecture:
- *Juan Ballesteros*, Novasite Pharmaceuticals, San Diego, CA, USA: Pharmacological engineering of challenging GPCR drugs (16:15-17:00)

Oral presentations:
- *Thomas Högberg*, 7TM Pharma, Hørsholm, Denmark: A physicogenetic method to assign ligand-binding relationsships between 7TM receptors applied on CRTH2 (17:00-17:15)
- *Patrick Page*, Serono Pharmaceutical Research Institute, Geneva, Switzerland: First non prostaglandin-like small molecule antagonists of the prostanoid FP receptor: Design, synthesis and pharmacological evaluation of potent, selective, orally active prostaglandin F2 receptor antagonists (17:15-17:30)

TUESDAY

				Starting time
Philip S. Portoghese, University of Minnesota, Minneapolis, MN, USA Ligands that selectively target heterodimeric opioid receptors Chairman: *Hans Bräuner-Osborne*				9:00
Exhibition and coffee				9:45
CNS II depression & anxiety	**Receptors II GPCRs structure & ligands**	**Oligosaccharides as therapeutics**	**Enzymes III new targets**	10:30
Poster session (posters with even numbers) - Lunch				12:30
Receptors III ionotropic structure & ligands	**CNS III epileptic disorders**	**Inflammation**	**Molecular docking, scoring and virtual screening**	14:30
Coffee				16:30
Nauta Award Lecture: *Robin Ganellin*, The University College of London, UK How to generate drug leads in the absence of high throughput screening (HTS) Chairman: *Ferran Sanz*				17:00 (17:45 End)

Session 4A CNS II: depression and anxiety
Chairman: *Klaus Bøgesø*, H. Lundbeck, Valby, Denmark
Key lectures:
- *Sandra Hogg*, H. Lundbeck, Valby, Denmark: Current trends in antidepressant and anxiolytic research (10:30-11:15)
- *David Tattersall*, Merck Sharp and Dohme, Harlow, UK: NK1 receptor antagonists: treatments for a variety of diseases? (11:15-12:00)

Oral presentations:
- *Magnus W. Walter*, Eli Lilly, Surrey, UK: Novel selective norepinephrine re-uptake inhibitors (12:00-12:15)
- *J. Ignacio Andrés*, Johnson & Johnson Pharmaceutical R&D, Toledo, Spain: The discovery of a new series of centrally active tricyclic isoxazoles combining 5-HT reuptake inhibition with alpha2-adrenoceptor blocking activity (12:15-12:30)

Session 4B Receptors II: GPCRs - structure & ligands
Chairman: *Henk Timmerman*, Vrije Universiteit, Amsterdam, The Netherlands
Key lectures:
- *Graeme Milligan*, University of Glasgow, Glasgow, UK: The basis and selectivity of the dimerisation of G protein-coupled receptors (10:30-11:15)
- *Nigel Birdsall*, National Institute of Medical Research, London, UK: Novel pharmacological aspects of the allosteric regulation of binding and function at GPCRs (11:15-12:00)

Oral presentations:
- *Aldo Jongejan*, Vrije Universiteit, Amsterdam, The Netherlands: Activation of aminergic GPCRs: insights from the histamine H1 receptor (12:00-12:15)
- *Peter Gmeiner*, Friedrich-Alexander University, Erlangen, Germany: Interactive studies on GPCR modeling, ligand synthesis and pharmacological investigations including site directed mutagenesis to understand dopamine receptor subtype selectivity, ligand efficacy and binding modes (12:15-12:30)

Session 4C Oligosaccharides as therapeutics
Chairman: *Klaus Bock*, The Carlsberg Laboratory, Valby, Denmark
Key lectures:
- *Mark von Itzstein*, Griffith University, Queensland, Australia: Exploring sialic acid recognising proteins as drug discovery targets (10:30-11:15)
- *Ole Hindsgaul*, The Carlsberg Laboratory, Valby, Denmark: The chemical challenge of converting weak oligosaccharide ligands into potent inhibitors (11:15-12:00)

Oral presentations:
- *João P. A. Neres*, University of Manchester, Manchester, UK: Design of inhibitors for Trypanosoma cruzi trans-sialidases (12:00-12:15)
- *Lidia A. Baltina*, Institute of Organic Chemistry Ufa Research Centre of RAS, Ufa, Russia: Design and synthesis of novel glycyrrizic acid derivatives and analogues with positive antiviral activity (12:15-12:30)

Session 4D Enzymes III: new targets
Chairman: *Rolf W. Hartmann*, Saarland University, Saarbruecken, Germany
Key lectures:
- *Donald Poirier*, Centre Hospitalier Universitaire de Québec, Sainte-Foy, Québec, Canada: Solution and solid phase synthesis of inhibitors of steroid sulfatase, 17ß-HSD type 1 and 17ß-HSD type 3, three key enzymes of estrogen and androgen biosynthesis (10:30-11:15)
- *Rolf W. Hartmann*, Saarland University, Saarbruecken, Germany: Discovery of potent and selective inhibitors of human aldosterone synthase (CYP11B2) - a new target for the treatment of congestive heart failure and myocardial fibrosis (11:15-12:00)

Oral presentations:
- *Jean-Pierre Gotteland*, Serono Pharmaceutical Research Institute, Geneva, Switzerland: Design and synthesis of novel, potent, selective and in vivo active inhibitors of the c-Jun-N-terminal Kinase (JNK) (12:00-12:15)
- *Jens-Uwe Peters*, F. Hoffmann-La Roche, Basel, Switzerland: Rapid improvement of activity and compound properties in a series of novel DPP-IV inhibitors during the Hit-to-Lead process (12:15-12:30)

Session 5A Receptors III: ionotropic - structure & ligands
Chairman: *Jan Egebjerg*, H. Lundbeck, Valby, Denmark
Key lectures:
- *Bente Frølund*, The Danish University of Pharmaceutical Sciences, Copenhagen, Denmark: Ligands for the GABAA receptor: Structure-activity relationships (14:30-15:15)
- *August B. Smit*, Vrije Universiteit, Amsterdam, The Netherlands: Acetylcholine binding protein (AChBP) from synaptic modulation to a high-resolution model for the extracellular domain of ligand gated ion channels (15:15-16:00)

Oral presentations:
- *Rohan J. Kumar*, University of Sydney, Australia: Cyclopentene phosphinic acids as GABAC selective antagonists (16:00-16:15)
- *Scott R. Breining*,Targacept, Winston-Salem, NC, USA: The alpha-methyl metanicotines: Nicotinic acetylcholine receptor modulators for treatment of CNS disorders (16:15-16:30)

Session 5B CNS III: epileptic disorders
Chairman: *Richard B. Silverman*, Northwestern University, Evanston, IL, USA
Key lectures:
- *David Wustrow*, Pfizer, Ann Arbor, MI, USA: Correlation of In Vitro and In Vivo effects of pregabalin and structurally-related compounds (14:30-15:15)
- *Benoît Kenda*, UCB, Braine-l'Alleud, Belgium: Discovery of ucb 34714: a new pyrrolidone derivative with antiepileptic properties (15:15-16:00)

Oral presentations:
- *Sándor Sólyom*, IVAX Drug Research Institute, Budapest, Hungary: A new class of AMPA antagonist 2,3-Benzodiazepines (16:00-16:15)
- *Eleonora Ghidini*, Chiesi Farmaceutici, Parma, Italy: Preparation and anticonvulsant activity of a series of functionalized amino acids with tetralinyl and indanyl moieties (16:15-16:30)

Session 5C Inflammation
Chairman: *Peter Ettmayer*, Novartis Research Institut, Vienna, Austria
Key lectures:
- *Berndt Oberhauser*, Novartis Research Institut, Vienna, Austria: Low-molecular-weight inhibitors of integrin binding and signalling (14:30-15:15)
- *Richard Horuk*, Berlex Biosciences, Richmond, CA, USA: Chemokine receptor antagonists (15:15-16:00)

Oral presentations:
- *John C. McKew*, Wyeth Research, Cambridge, MA, USA: Discovery of a new class of anti-inflammatory: Indole cPLA2 sinhibitors (16:00-16:15)
- *Claudio Sturino*, Merck Frosst Centre for Therapeutic Research, Pointe Claire-Dorval, Quebec, Canada: The development of L-888839, a highly potent and selective prostaglandin D2 receptor antagonist: lessons in reactive intermediates and transporters (16:15-16:30)

Session 5D Molecular docking, scoring and virtual screening
Chairman: *Tommy Liljefors*, The Danish University of Pharmaceutical Sciences, Copenhagen, Denmark
Key lectures:
- *Christopher W. Murray*, Astex Technology, Cambridge, UK: Virtual and crystallographic screening of low molecular weight compounds (14:30-15:15)
- *Tanja Schulz-Gasch*, F. Hoffmann-La Roche, Basel, Switzerland: Virtual screening and structure-based design (15:15-16:00)

Oral presentations:
- *Micael Jacobsson*: Biovitrum & Uppsala University, Sweden: Multivariate statistical analysis of docking scores in structure-based virtual screening (16:00-16:15)
- *Theodora Steindl*, University of Innsbruck, Innsbruck, Austria: Pharmacophore modelling and docking studies: The search for new HRV coat protein inhibitors (16:15-16:30)

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WEDNESDAY – Malmö	Starting time
Buses to Malmoe	8:45
Coffee at Slagthuset	10:00
UCB Award Lecture: *Jesper Wengel*, The University of Southern Denmark, Odense, Denmark LNA (locked nucleic acid) and functionalized nucleic acids: towards efficient gene silencing and optimised nucleic acid based therapeutics Chairman: *Ferran Sanz*	10:30
AFMC Lecture: *Yoshichika Arakawa*, National Institute of Infectious Diseases, Tokyo, Japan Lateral transfer of genetic determinants for multi-drug resistance to clinically important bacilli Chairman: *Henk Timmerman*	11:15
Lunch	12:00
Stan van Boeckel, Organon, Oss, The Netherlands From the bench to production chemistry - what about complex molecules Chairman: *Klaus Gundertofte*	13:00
Klaus Müller, F. Hoffmann-La Roche, Basel, Switzerland Structure-based drug discovery Chairman: *Tommy Liljefors*	13:45 (14:30 End)
Free activities in Malmoe	
Get together in Malmoe	18:00
Train for Copenhagen	

THURSDAY				
John Dixon, AstraZeneca, Charnwood, UK Pharmacokinetics and drug discovery Chairman: *Anders Karlén*				9:00
Exhibition and coffee				9:45
ADME and toxicology	**CNS IV neurodegenerative disorders**	**Diabetes new aspects**	**Receptors IV nuclear structure & ligands**	10:30
Poster session (all posters) - Lunch				11:45
Obesity disorders	**Sleep disorders new targets**	**Receptors V orphan structure & ligands**	**ADME and drug design**	13:30
Coffee				14:45
Stuart R. Walker, CMR International, Surrey, UK The future of the pharma industry Chairman: *Henk Timmerman*				15:15
Closing of symposium and welcome to ISMC2006 *Povl Krogsgaard-Larsen*, Chairman *Fethi Sahin*, Gazi University, Ankara, Turkey				16:00 (16:15 End)

Session 6A ADME and toxicology
Chairman: *Bernard Testa*, University Hospital Centre, Lausanne, Switzerland
Key lecture:
- *Jean-Michel Scherrmann*, INSERM, Hôpital Fernand WIDAL, Paris, France: Expression and functional role of multidrug resistance transporters at the blood-brain barrier (10:30-11:15)

Oral presentations:
- *Markku D. Hämäläinen*, Biacore, Uppsala, Sweden: Characterisation of thrombin leads with the new Biacore S51® - Identification of potent binders with favourable early ADME-properties (11:15-11:30)
- *Jon Våbenø*, University of Tromsø, Norway: Ketomethylene based dipeptidomimetics as pro-moieties for hPEPT1 targeted prodrugs (11:30-11:45)

Session 6B CNS IV: neurodegenerative disorders
Chairman: *Patrice Talaga*, UCB S.A., Braine-l'Alleud, Belgium
Key lecture:
- *Tim Harrison*, Merck Sharp & Dohme Research Laboratories, Harlow, UK: Gamma-secretase as a target for drug intervention in alzheimer's disease (10:30-11:15)

Oral presentations:
- *Kouji Hattori*, Fujisawa Pharmaceutical, Osaka, Japan: Rational approaches to discovery of orally active & brain penetrable PARP inhibitors (11:15-11:30)
- *Akgül Yesilada*, Hacettepe University, Ankara, Turkey: New Naproxen derivatives: Synthesis and screening of antiinflammatory, analgesic and anti-aggregation effects on ß-amyloid(1-40) peptide (11:30-11:45)

Session 6C Diabetes: new aspects
Chairman: *John Bondo Hansen*, Novo Nordisk, Måløv, Denmark
Key lecture:
- *Jens Juul Holst*, University of Copenhagen, Copenhagen, Denmark: Incretin action as the basis for treatment of type 2 diabetes (10:30-11:15)

Oral presentations:
- *Guido Kurz*, Biovitrum, Stockholm, Sweden: For mice and men? Inhibitors of 11beta-hydroxysteroid dehydrogenase type 1 with anti-diabetic potential (11:15-11:30)
- *Daniel D. Sternbach*, GlaxoSmithKline R&D, Research Triangle Park, NC, USA: Synthesis and crystal structure of a PPARpan agonist that delivers glycemic control and improved lipid profiles without weight gain (11:30-11:45)

Session 6D Receptors IV: nuclear - structure & ligands
Chairman: *Dirk Leysen*, Devgen nv, Ghent-Zwijnaarde, Belgium
Key lectures:
- *Peter Thomas*, University of Texas at Austin, Port Aransas, TX, USA: The discovery and characterization of a new family of cDNAs encoding progestin membrane receptors in vertebrates (10:30-11:15)
- *Jan-Åke Gustafsson*, Karolinska Institutet, Huddinge, Sweden: Recent excitements in drug development based on novel insights in estrogen signaling (11:15-12:00)

Session 7A Obesity disorders (ACS session)
Chairman: *Paul Ornstein*, Eli Lilly, Indianapolis, IN, USA
Key lectures:
- *Andrew J. Carpenter*, GlaxoSmithKline, Research Triangle Park, NC, USA: The discovery of potent and selective MCH receptor-1 antagonists for the treatment of obesity (13:30-14:00)
- *Matthew J. Fisher*, Eli Lilly, Indianapolis, IN, USA: Discovery of ligands for melanocortin receptors (14:00-14.30)
- *Kevin W. Gillman*, Bristol-Myers Squibb Company, Wallingford, CT, USA: Selective NPY5 antagonists as potential therapeutic agents for obesity (14:30-15:00)

Session 7B Sleep disorders: new targets
Chairman: *Bjarke Ebert*, H. Lundbeck, Valby, Denmark
Key lectures:
- *Bjarke Ebert*, H. Lundbeck, Valby, Denmark: Functional selectivity of GABAA receptor agonists: a possibility for novel drugs! (13:30-14:15)
- *Francesca Stingele*, Neurim Pharmaceuticals, Lausanne, Switzerland: Circadin - 2mg prolonged release melatonin: a new treatment paradigm improving quality of sleep (14:15-15:00)

Session 7C Receptors V: orphan - structure & ligands
Chairman: *Hans Bräuner-Osborne*, The Danish University of Pharmaceutical Sciences, Copenhagen, Denmark
Key lecture:
- *Mark Fidock*, Pfizer, Sandwich, Kent, UK: Functional validation of newly paired orphan GPCRs (13:30-14:15)

Oral presentation:
- *Petrine Wellendorph*, The Danish University of Pharmaceutical Sciences, Copenhagen, Denmark: Deorphanization of GPRC6A – a novel human family C G-protein coupled receptor (14:15-14:45)

Session 7D ADME and drug design
Chairman: *Kristina Luthman*, Göteborg University, Göteborg, Sweden
Key lecture:
- *Christopher A Lipinski*, Pfizer Global R&D, Groton Labs (retired), Groton, CT, USA: Solubility, permeability and drug-likeness: why chemistry is important (13:30-14:15)

Oral presentations:
- *Christel A. S. Bergström*, Uppsala University, Sweden: A model for the prediction of aqueous solubility and intestinal absorption (14:15-14:30)
- *Marco Pintore*, BioChemics Consulting, Orleans Cedex 2, France: Predicting ADME properties by Radial Basis Functions (RBF) (14:30-14:45)

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SOCIAL EVENTS

Welcome Reception and Registration
Sunday, August 15, at 19:30 hrs at Symposium Venue – Bella Center – the Exhibition Area.
Included in the registration fee for delegates and accompanying persons.

Get Together in Malmö
Wednesday, August 18, at 18:00 hrs.
Buffet, Swedish snap songs and entertainment at Slagthuset, the venue of the lectures the day in Sweden. Transportation by bus and train.
Included in the registration fee for delegates and accompanying persons.
Tickets for the trip back, by train, you will get when entering the bus for Malmoe.

Optional social event
Monday, August 16
Concert by Michala Petri, flute, and Lars Hannibal, guitar, at Holmens Kirke and Buffet at Børsen at 19:00 hrs.
Price DKK 645.
Registration is mandatory.

EXHIBITORS

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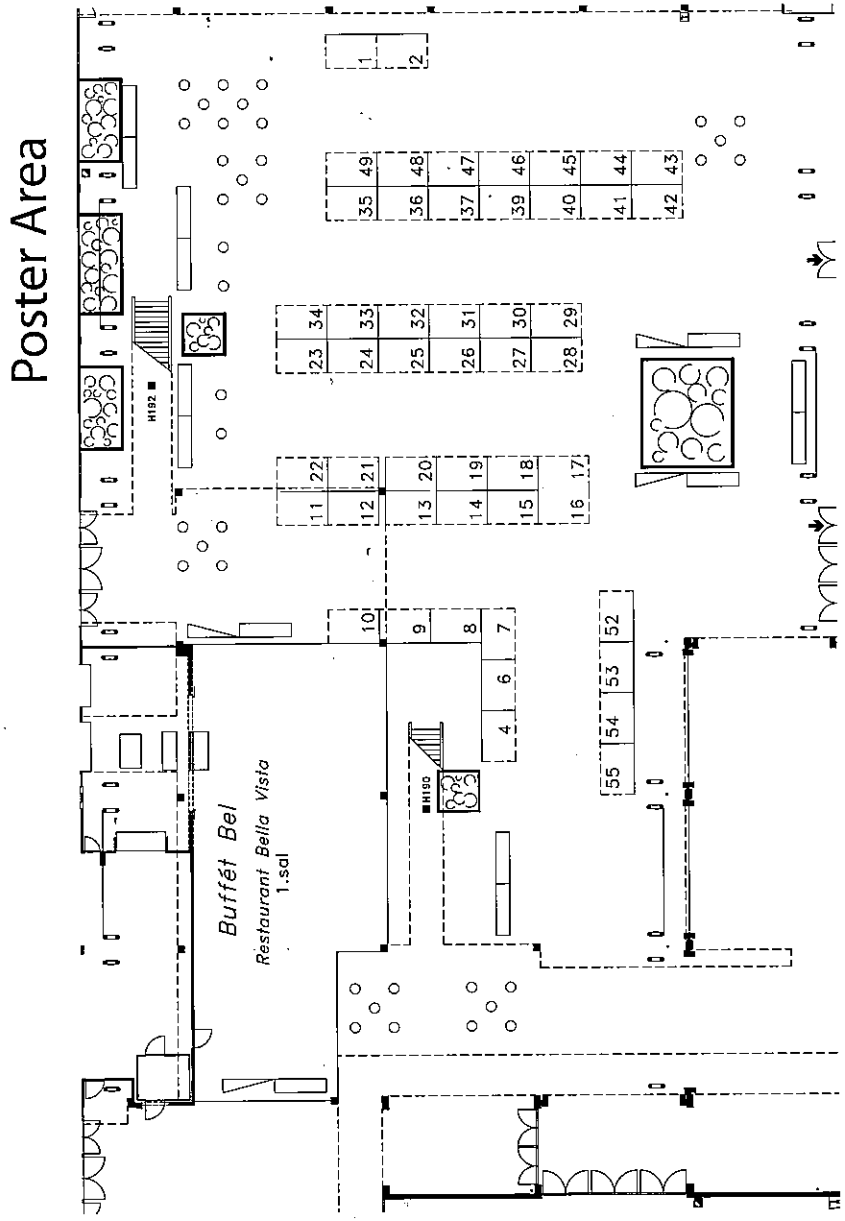

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Albany Molecular Research, Inc. (Nasdaq: AMRI) is a leading chemistry-based drug discovery, development, and manufacturing company. AMRI's comprehensive technologies include diverse lead-seeking libraries, medicinal and combinatorial chemistry, CADD, chemical and bioprocess development, high-throughput screening, and cGMP manufacturing. The company works with many leading pharmaceutical and biotechnology companies. 26
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Argenta Discovery Limited 25
Richard Lingard, Vice President, Business Development. Dr Anthony Baxter, CEO
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Argenta discovery is a leading hit finding, lead optimisation and pre-clinical candidate discovery company. Our unique integrated approach to drug discovery is based on the highest quality medicinal chemistry, biochemistry and eADME capabilities. We place a premium on the experience and successful track record of our staff. We have a pipeline of pre-clinical candidates which are available for sale or licence including our Histone Deacetylase Inhibitor (HDACi, oncology) programme and our Prostaglandin E2 agonist (EP-2, bone resporption) programme. In addition, we have 4 further therapeutic programmes at lead optimisation stage. We also offer contract research services in medicinal chemistry and biochemistry for both major pharma and biotech customers.

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ASINEX is a full-service chemistry provider of 'Intelligent Chemistry' for the lead generation and optimization stage of drug discovery. Well known as a supplier of diverse, small molecule libraries for screening and building blocks for combinatorial chemistry, ASINEX has developed a reputation for cost-effective and efficient lead optimization, custom synthesis and focused library generation. Based in Moscow, with a total of 104 organic chemists (41 Ph.D.), 8 computational chemists (6 Ph.D.) and 17 biologists (11 Ph.D.), ASINEX has powerful drug discovery resources. 29

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Chemical Computing Group's product MOE (Molecular Operating Environment) contains a broad range of drug discovery and molecular modelling applications for workstations, desktop and laptop machines running UNIX, Linux, Windows and Mac OS/X, including protein structural modelling and display, pharmacophore derivation and search, small molecule modelling and database applications. 7

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Our staff looks forward to meeting you there. 44
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16&17

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Contents

Volume 1. **General Principles of Medicinal Chemistry**, Peter Kennewell, BBSRC, Swindon, UK
Volume 2. **Strategy and Drug Research**, Walter Moos, Mitokor, San Diego, USA
Volume 3. **Technologies of Drug Discovery**, Hugo Kubinyi, University of Heidelberg, Germany
Volume 4. **Computer-aided Drug Design**, Jonathan Mason, Pfizer, Sandwich, UK
Volume 5. **ADMET**, Bernard Testa, University Hospital Centre (CHUV), Lausanne, Switzerland; Han van de Waterbeemd, Pfizer, Sandwich, UK
Volume 6. **Therapeutic Areas - I**, Mike Williams, Northwestern University, Chicago, USA
Volume 7. **Therapeutic Areas - II**, Jacob Plattner, Anacor Pharmaceuticals, Palo Alto, USA and Manoj Desaj, Gilead Sciences, Foster City, USA
Volume 8. **Case Histories and Cumulative Index.**

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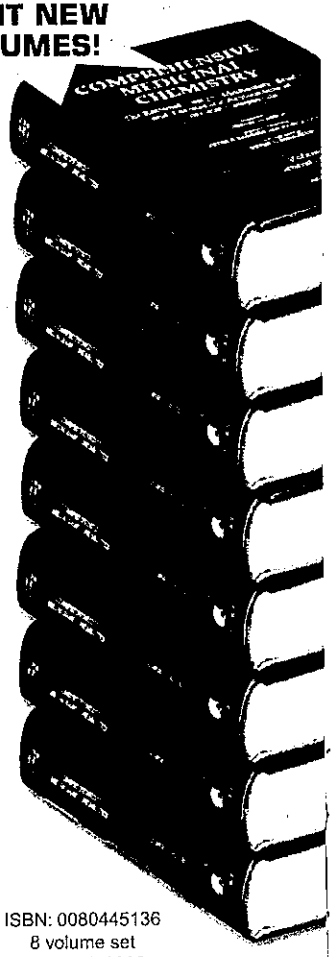

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Drugs of Natural Origin

A Textbook in Pharmacognosy, 5th revised edition
by Gunnar Samuelsson

Previous editions of Drugs of Natural Origin have been well received. The book is recognised and appreciated as a valuable textbook in pharmacognosy for undergraduate and graduate studies at universities in many countries throughout the world. The 3rd English edition was translated into Italian as well as Greek. It is now a pleasure to present the enlarged and longed for 5th edition.

About forty percent of the drugs currently used are derived from natural sources. Most are pure substances which are isolated from various organisms and used directely or after modification. This book describes the origin of such compounds, their chemistry and biochemistry as well as their employment in medicine. The material is arranged according to biosynthetic principles, a unique feature which places the substances in a natural context and facilitates understanding and learning of the often complicated chemical structure.

Preface to the 5th edition

Although only 3 years has passed since the the 4th edition of this book was published, an extensive revision was called upon by the fast development in the field. This is particularly true for polyketide antibiotics which have been subject to intensive research activities resulting in the elucidation of biosynthetic pathways and characterization of the large enzymes involved. Modern molecular biology techniques have played an extensive role in this development. Based on these findings it is now possible to construct new molecules with different pharmacological activities which can be developed into new and better drugs.

The non-mevalonate pathway for the biosynthesis of isoprenoids has turned out to be of much greater importance than originally realized. This has necessitated rewriting of the corresponding parts of the book. Also newly published information on the biosynthesis of artemisinin, ginkgolides and paclitaxel has been included.

The biosynthesis of the important antibiotic vancomycin has now been elucidated at the genetic and enzymatic level and the information has been included in the book as it is a very important development in the field of antibiotics which opens up new possibilities for construction of new compounds, greatly needed in the never ceasing battle against antibiotic-resistant strains of bacteria.

The giant work on the biosynthesis of coenzyme B12 has continued and the new findings have been included in chapter 12.

Finally, a long overdue revision of the text concerning the dark reactions in photosynthesis (chapter 4) has been performed. Also the biosynthesis of sucrose has been revised and a paragraph on the biosynthesis of starch has been added.

As for the previous editions I am indepted to the publishers – the Swedish Pharmaceutical Press – for excellent production of the book and for a very good cooperation in the process of publishing.

Rimforsa, March 2004 Gunnar Samuelsson

620 pages, illustrated in colour, ISBN 91 9743 184 2
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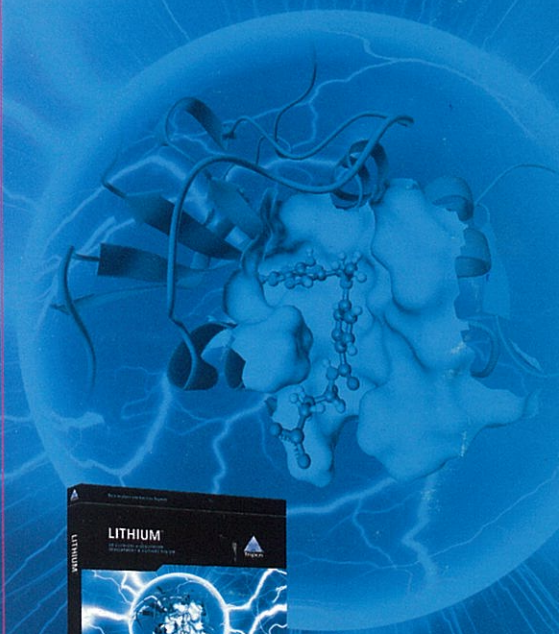

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