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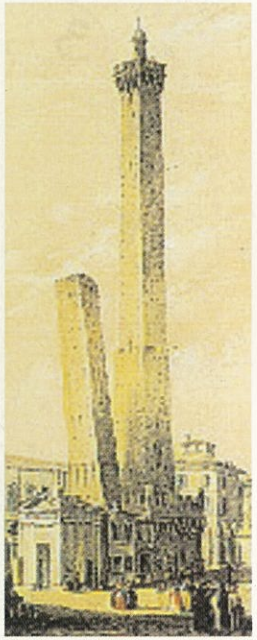

XVIth International Symposium on Medicinal Chemistry

Bologna, Italy
September 18 - 22, 2000
Palazzo della Cultura e dei Congressi

Università degli Studi di Bologna

B O L O G N A
Città Europea della Cultura

FINAL PROGRAMME

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P

LAST MINUTE CHANGES

1. SCIENTIFIC PROGRAMME

Tuesday, September 19, 2000

PL1 (9.00-9.45, Europauditorium) by R.R. Ruffolo will be replaced by:

"GABA and glutamate receptor ligands. Design, discovery and therapeutic aspects"
P. Krogsgaard-Larsen (Copenhagen, Denmark)

Wednesday, September 20, 2000

OC6 (12.30-12.45, Sala Italia) will be delivered by *O.N. Voskresensky*

Thursday, September 21, 2000

ML39 (10.30-10.55, Europauditorium) will be delivered by *J.-C. Rochet* (Boston, MA, USA)

ML42 (14.30-14.55, Europauditorium) will be delivered by *J.-M. Vernier* (La Jolla, CA, USA)

PB-157: "In silico HTS tests for CNS Penetration" *G.M. Keseru* et al. (Budapest, Hungary)

PA-49 will be discussed as PB-158

PB-159: "Directed library synthesis for kinase targets" *M. Coombs* et al. (Loughborough, UK)

PB-160: "Directed library approach to lead generation libraries" *S. King* (Loughborough, UK)

PB-161: "Exploring the possibilities of combinatorial biosynthesis anthracyclines"
T. Kunnari et al. (Galilaeus Oy, Finland)

Friday, September 22, 2000

PL3 (9.00-9.45, Europauditorium) will be delivered by *D.G. Trist* (Verona, Italy)

PC-159: "Protease inhibitors as antiviral drugs for the treatment of dengue virus infections"
D. Leung et al. (Queensland, Australia)

PB-139 will be discussed as PC-160

PC-161: "The discovery of dual D_2-receptor and $ß_2$-adrenoceptor agonists for the treatment of airway diseases"
R.V. Bonnert et al. (Loughborough, UK)

PC-162: High throughput measurements and prediction of physico chemical parameters to predict absorption, an integrated approach" *C. Peake*, (Forest Row, East Sussex, UK)

2. SPONSORS

The Organizing Committee wishes to thank the companies and the organizations that have supported the Symposium. A complete list of sponsors is included in the Final Programme.
The following companies have also supported the Symposium:

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Cambridge Discovery Chemistry has withdrawn its support.

GABA AND GLUTAMATE RECEPTOR LIGANDS. DESIGN, DISCOVERY AND THERAPEUTIC ASPECTS

Povl Krogsgaard-Larsen
Department of Medicinal Chemistry
The Royal Danish School of Pharmacy
2 Universitetsparken
Copenhagen, Denmark

4-Aminobutyric acid (GABA) and glutamic acid (Glu) are the major central inhibitory and excitatory neurotransmitters, respectively. Most, if not all, neurones in the CNS are under the control of these transmitter amino acids, both of which have been implicated in a number of psychiatric and neurological disorders. GABA as well as Glu operate through multiple ionotropic and metabotropic receptors, all of which are potential targets for therapeutic intervention. The ionotropic GABA ($GABA_A$ and $GABA_C$) and Glu (NMDA, AMPA and kainic acid) receptors are heteromeric receptors comprising different subunits, and in addition to the transmitter recognition site(s), most of these receptors contain allosteric or regulatory sites of pharmacological interest. Ligands acting at the receptor recognition sites are frequently designed using naturally occurring compounds as leads or by bioisosteric modification of the endogenous ligands, and these approaches have led to a variety of subtype-selective pharmacological tools and potential drugs. Ligands at additional receptor binding sites are typically discovered accidentally, and although such binding sites may not have any physiological function, such ligands may have considerable therapeutic interest. It is likely that receptor subtype-specific ligands will be identified within this category of compounds.

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SCIENTIFIC PROGRAMME

Monday, September 18, 2000

15.00-17.00	Registration	
17.00-17.30	Opening Cerimony Presentation of the Nauta Award	Europauditoriu
17.30-18.30	Inaugural Lecture (IL) Chairman: *P.S. Portoghese (Minneapolis, MN, USA)* **Rational drug design. What will it look like at the end of the 21st Century?** *D. Rich (Madison, WI, USA)*	
18.30-20.30	**Welcome Cocktail Party**	

Tuesday, September 19, 2000

8.00-9.00	Registration	
9.00-9.45	Plenary Lecture (PL1) Chairman: *A. Leonardi (Milan, Italy)* **Pharmacotherapy of the major cardiovascular diseases** *R.R. Ruffolo (King of Prussia, PA,USA)*	Europauditorium
Theme 1	**Antihypertensive Agents** Chairman: *A. Leonardi (Milan, Italy)*	Sala Italia
10.00-10.25	Main Lecture (ML1) **Applying modern technologies to research in hypertension: a promise for better drugs?** *G. Gaviraghi (Verona, Italy)*	
10.30-11.00	Coffee Break	
11.00-11.25	Main Lecture (ML2) **Design, discovery, and pharmacology of the vasopeptidase inhibitor Vanlev™: a novel agent for the treatment of hypertension and congestive heart failure** *J.A. Robl (Princeton, NJ,USA)*	
11.30-11.55	Main Lecture (ML3) **The emerging pathophysiological significance of endothelin in cardiovascular disease** *J.D. Elliott (King of Prussia, PA, USA)*	
12.00-12.25	Main Lecture (ML4) **Piperidine renin inhibitors: from leads to drug candidates** *H.P. Märki (Basel, Switzerland)*	
12.30-12.45	Oral Communication (OC1) **Phenylalkynes: a new class of thrombin and factor Xa inhibitors** *H.W.M. Priepke (Biberach an der Riss, Germany)*	

Tuesday, September 19, 2000

Theme 2	**The Impact of Organic Chemistry on Drug Discovery** Chairmen: *D.L. Boger (La Jolla, CA, USA)* *C. Chatgilialoglu (Bologna, Italy)*	Europauditorium
10.00-10.25	Main Lecture (ML5) **Natural products and nature's lessons: five natural products and five solutions to the sequence selective recognition of duplex DNA** *D.L. Boger (La Jolla, CA, USA)*	
10.30-11.00	Coffee Break	
11.00-11.25	Main Lecture (ML6) **Synthesis of conformationally fixed nucleosides via radical cascade reactions** *C. Chatgilialoglu (Bologna, Italy)*	
11.30-11.55	Main Lecture (ML7) **Structure-based design of nonpeptide HIV protease inhibitors** *A.K. Ghosh (Chicago, IL, USA)*	
12.00-12.25	Main Lecture (ML8) **Transmembrane ion transport mediated by polyethers in a precise conformation** *J. Delgado Martin (Sevilla, Spain)*	
12.30-12.45	Oral Communication (OC2) **High pressure synthesis of enantiomerically pure pyrazole[3,4-*d*]pyrimidines** *R.J. Quinn (Brisbane, Australia)*	

Theme 3 **Antiinfective Agents** Sala Topazio
Chairman: *T. Kobayashi (Tokyo, Japan)*

10.00-10.25 Main Lecture (ML9)
Characterisation of inter- and intra-molecular interactions of the dengue virus RNA dependent RNA polymerase as potential drug targets
S.G. Vasudevan (Camberra, Australia)

10.30-11.00 Coffee Break

11.00-11.25 Main Lecture (ML10)
Recent advances in the field of quinolones
M. Takemura (Tokyo, Japan)

11.30-11.55 Main Lecture (ML11)
Design of new penem antibiotics based on β-lactam-interacting enzyme structures
M. Ishiguro (Osaka, Japan)

12.00-12.25 Main Lecture (ML12)
Discovery of Gemifloxacin (Factive, LB20304a): a quinolone of new generation
C.Y. Hong (Tae-Jon, Korea)

12.30-12.45 Oral Communication (OC3)
Identification of novel lipopeptides from Streptomyces *Griseus* TCA65 as inhibitors of bacterial leader peptidase
J.A. Hueso-Rodriguez (Tres Cantos, Spain)

12.50-14.00 Lunch Break

Theme 4 **Hypolipidemics/Antiatherosclerotics** Sala Topazio
Chairman: *D. Hickey (Harlow, Essex, , UK)*

14.00-14.25 Main Lecture (ML13)
The discovery of GW 328713: a novel inhibitor of apolipoprotein-B secretion
P. Martres (Les Ulis, France)

14.30-14.55 Main Lecture (ML14)
Lipoprotein-associated PLA_2 inhibition - A novel, non lipid lowering strategy for atherosclerosis therapy
C. Leach (Harlow, Essex, UK)

15.00-15.30 Coffee Break

15.30-15.55 Main Lecture (ML15)
The development of small molecule antagonists for the MCP-1 receptor
C. Tarby (Wilmington, DE, USA)

16.00-16.25 Main Lecture (ML16)
New carboline derivatives as inhibitors of the microsomal triglyceride transfer protein for the treatment of dyslipidemias: the discovery of implitapide
U. Müller (Wuppertal, Germany)

Tuesday, September 19, 2000

Theme 5	**Anticancer Agents** Chairmen: *M. Palumbo (Padua, Italy)* *N. Mongelli (Nerviano, Italy)*	Sala Italia
14.00-14.25	Main Lecture (ML17) **Telomeric DNA: a novel target for chemotherapeutic intervention** *S. Neidle (Sutton, Surrey UK)*	
14.30-14.55	Main Lecture (ML18) **The design of irreversible inhibitors of the erbB family of transmembrane receptors** *W.A. Denny (Auckland, New Zealand)*	
15.00-15.30	Coffee Break	
15.30-15.55	Main Lecture (ML19) **Antisense and antigene strategies for the treatment of cancer** *C. Hélène (Paris, France)*	
16.00-16.25	Main Lecture (ML20) **A new class of cytotoxic DNA minor groove binders, alpha-halogenoacrylic derivatives of pyrrolecarbamoyl oligomers** *P. Cozzi (Nerviano (MI), Italy)*	

Tuesday, September 19, 2000

Theme 6	**New Paradigms in Receptorology** Chairman: *H. Timmerman (Amsterdam, The Netherlands)*	Europauditoriu
14.00-14.25	Main Lecture (ML21) **Virus-induced GPCRs: a new target for drug development** *M.J. Smit (Amsterdam, The Netherlands)*	
14.30-14.55	Main Lecture (ML22) **Molecular mechanisms of agonist-receptor interaction leading to activation** *H. Weinstein (New York, NY, USA)*	
15.00-15.30	Coffee Break	
15.30-15.55	Main Lecture (ML23) **Allosteric modulation of G protein-coupled receptors** *A.P. IJzerman (Leiden, The Netherlands)*	
16.00-16.25	Main Lecture (ML24) **Functional consequences of genetic variation in β_1 and β_2 adrenoceptors in the human population** *S.B. Liggett (Cincinnati, OH, USA)*	
16.30-18.00	**Poster Session A**	Foyer
	Exhibition	
21.00-22.30	**Concert** (Chiesa dei Servi, Strada Maggiore)	

9.00-9.45	Plenary Lecture (PL2) Chairman: *T. J. Perun (Hempstead, TX, USA)* **New developments in antiviral chemotherapy** *E. De Clercq (Belgium)*	Europauditorium

Theme 7 — **Ligands for P_1 and P_2 Purinergic Receptors** — Sala Topazio

Chairmen: *P.G. Baraldi (Ferrara, Italy)*
K.A. Jacobson (Bethesda, MD, USA)

10.00-10.25	Main Lecture (ML25) **Structurally-related nucleotides as selective agonists and antagonists at $P2Y_1$ receptors** *K.A. Jacobson (Bethesda, MD, USA)*
10.30-11.00	Coffee Break
11.00-11.25	Main Lecture (ML26) **Selective A_{2A} adenosine receptor antagonists** *E. Ongini (Milan, Italy)*
11.30-11.55	Main Lecture (ML27) **A_1 Adenosine receptors and their ligands: overview and recent developments** *C.E. Müller (Bonn, Germany)*
12.00-12.25	Main Lecture (ML28) **New ligands at adenosine (P_1) receptors** *L.J.S. Knutsen (Winnersh, Berkshire, UK)*
12.30-12.45	Oral Communication (OC4) **New structure-activity relationships of P_2-receptor antagonists structurally related to reactive blue 2** *M. Glänzel (Freiburg, Germany)*

Theme 8 — **Antiviral Agents** — Europauditoriu

Chairman: *J.D. Rodgers (Wilmington, DE, USA)*

10.00-10.25	Main Lecture (ML29) **Covalent and non-covalent inhibitors of HCV NS3 protease** *V.G. Matassa (Pomezia, Italy)*
10.30-11.00	Coffee Break
11.00-11.25	Main Lecture (ML30) **Second generation NNRTIs active against clinically relevant mutant variants of HIV-1 containing K103N** *S.K. Erickson-Viitanen (Wilmington, DE, USA)*
11.30-11.55	Main Lecture (ML31) **Inhibitors of viral mediated fusion** *D.M. Lambert (Durham, NC, USA)*
12.00-12.25	Main Lecture (ML32) **Inhibitors of HIV integrase: antiviral activity and mechanism** *D. Hazuda (West Point, PA, USA)*
12.30-12.45	Oral Communication (OC5) **New approach to the synthesis of amino acid phosphoramidates of AZT** *J. Baraniak (Lodz, Poland)*

Wednesday, September 20, 2000

Theme 9	Natural Products Chairman: *K. Wright (Wallingford, CT, USA)*	Sala Italia
10.00-10.25	Main Lecture (ML33) **Combinatorial biosynthesis: new tools for the medicinal chemist** *C. Khosla (Stanford, CA, USA)*	
10.30-11.00	Coffee Break	
11.00-11.25	Main Lecture (ML34) **Inhibitors of efflux pump mediated drug resistance from microbial fermentation** *M.D. Lee (Mountain View, CA, USA)*	
11.30-11.55	Main Lecture (ML35) **Marine microorganisms: a major, new resource for drug discovery** *W. Fenical (La Jolla, CA, USA)*	
12.00-12.25	Main Lecture (ML36) **The potential of plants as a source of new drugs** *K. Hostettmann (Lausanne, Switzerland)*	
12.30-12.45	Oral Communication (OC6) **Natural flavonoids as a plentifull source of new drugs** *~~A.P. Levitsky~~ (Odessa, Ukraine)*	
12.50-14.00	**Lunch Break**	
	Excursions	

14:00-16:00 NC Meeting

Thursday, September 21, 2000

Theme 10	Neurodegenerative Diseases Chairmen: *F. Gualtieri (Florence, Italy)* *E. Kyburz (Zurich, Switzerland)*	Europauditoriu
9.00-9.25	Main Lecture (ML37) **Where do we stand with the pharmacological treatment of AD in the year 2000?** *E. Giacobini (Geneva, Switzerland)*	
9.30-9.55	Main Lecture (ML38) **Muscarinic agonists and antagonists in the treatment of Alzheimer's disease** *W. Greenlee (Kenilworth, NJ, USA)*	
10.00-10.30	Coffee Break	
10.30-10.55	Main Lecture (ML39) **Protein fibrillization: a possible therapeutic target for Alzheimer's and Parkinson's diseases** *P.T. ~~Lansbury~~ (Boston, MA, USA)* ROCHET	
11.00-11.25	Main Lecture (ML40) **Mechanisms of cell death in Parkinson's disease** *P. Jenner (London, UK)*	
11.30-11.45	Oral Communication (OC7) **Design, synthesis and biological activity of GPI6150, a novel PARP inhibitor** *V. Kalish (Baltimore, MD, USA)*	
11.50-12.05	Oral Communication (OC8) **Modeling of acetylcholinesterase inhibitors: huprine X, a novel high affinity inhibitor** *F.J. Luque (Barcelona, Spain)*	
12.10-12.25	Oral Communication (OC9) **Design and synthesis of conformationally restricted pyridylquinuclidines: the discovery of AR-R23465XX, a novel α_7 nicotinic agonist** *E. Phillips (Worcester, MA, USA)*	
12.30-14.00	Lunch Break	

14.00-14.25 Main Lecture (ML41)
Muscarinic agonists reduce CSF levels of amyloid β-peptides in patients with Alzheimer's disease
~~R.M. Nitsch~~ (Zurich, Switzerland)
Hoch ?

14.30-14.55 Main Lecture (ML42)
The discovery of selective nicotinic acetylcholine receptor agonists for the treatment of CNS disease
~~J. McDonald~~ (La Jolla, CA, USA)
S.M. VEENIER

15.00-15.30 Coffee Break

15.30-15.55 Main Lecture (ML43)
Novel, activity-dependent NMDA NR2B sybtype selective antagonist as neuroprotective agents
J.A. Kemp (Basel, Switzerland)

16.00-16.25 Main Lecture (ML44)
Inflammation and axonal regeneration after traumatic spinal cord injury: new ways of intervention
L. Schnell (Zurich, Switzerland)

Thursday, September 21, 2000

Theme 11 **Ligands for Glutamate and GABA Receptors** Sala Topazio
Chairmen: *W. Froestl (Zurich, Switzerland))*
R. Pellicciari (Perugia, Italy)

9.00-9.25 Main Lecture (ML45)
Metabotropic glutamate receptors: structure and new subtype selective ligands
R. Pellicciari (Perugia, Italy)

9.30-9.55 Main Lecture (ML46)
Novel mGluR ligands acting as glutamate carboxypeptidase II inhibitors; role as neuroprotective and anti-angiogenic agents
A.P. Kozikowski (Washington, DC, USA)

10.00-10.30 Coffee Break

10.30-10.55 Main Lecture (ML47)
Discovery and characterisation of non-competitive antagonists of group I metabotropic glutamate receptors
F. Gasparini (Basel, Switzerland)

11.00-11.25 Main Lecture (ML48)
Constrained amino acids as probes for the glutamate recognition site of group II metabotropic glutamate receptors
J.A. Monn (Indianapolis, IN, USA)

12.30-14.00 Lunch Break

14.00-14.25 Main Lecture (ML49)
Novel ligands for the GABA-A benzodiazepine binding site
A.M. MacLeod (Harlow, Essex, UK)

14.30-14.55 Main Lecture (ML50)
Ligands for expression cloning and isolation of $GABA_B$ receptors
W. Froestl (Basel, Switzerland)

15.00-15.30 Coffee Break

15.30-15.55 Main Lecture (ML51)
Structurally novel AMPA potentiators: new opportunities for drug development
P.L. Ornstein (Indianapolis, IN, USA)

16.00-16.25 Main Lecture (ML52)
Orally active subtype-selective NMDA receptor antagonists for the treatment of Parkinson's disease
J. Wright (Ann Arbor, MI, USA)

Thursday, September 21, 2000

Theme 12 **Pain and Inflammation** Sala Italia
Chairmen: *D. Donati (Verona, Italy)*
M. Pinza (Pomezia, Italy)

9.00-9.25 Main Lecture (ML53)
Progress and future trend in the cyclooxygenase-2 inhibitors area
P. Prasit (Dorval, Quebec, Canada)

9.30-9.55 Main Lecture (ML54)
Regulatory mechanisms of inflammatory cytokines as targets for drug design
A. Mantovani (Brescia, Italy)

10.00-10.30 Coffee Break

10.30-10.55 Main Lecture (ML55)
Novel bone antiresorptive agents which selectively inhibit the osteoclast vacuolar V-H^+-ATPase
C. Farina (Baranzate, Italy)

11.00-11.25 Main Lecture (ML56)
Disease modifying anti-osteoarthritic drugs: current therapies and new prospects around protease inhibition
G. De Nanteuil (Suresnes, France)

11.30-11.45 Oral Communication (OC10)
Ketone based inhibitors of cysteine proteases
R.W. Marquis (King of Prussia, PA, USA)

11.50-12.05 Oral Communication (OC11)
ML 3000, a non-redox dual inhibitor of cyclooxygenase and 5-lipoxygenase
S. Laufer (Blaubeuren, Germany)

12.10-12.25 Oral Communication (OC12)
Development of k-selective opioid agonists: optimization of 3,7-diazabicyclo[3.3.1]nonanones
U. Holzgrabe (Würzburg, Germany)

12.30-14.00 Lunch Break

14.00-14.25	Main Lecture (ML57) **Novel glycine antagonists as potent antihyperalgesic agents** *R. Di Fabio (Verona, Italy)*	
14.30-14.55	Main Lecture (ML58) **Inhibitors of sensory nerve sodium channels for the treatment of chronic pain** *M. Nobbs (Stevenage, Hertfordshire, UK)*	
15.00-15.30	Coffee Break	
15.30-15.55	Main Lecture (ML59) **Selective delta opioid receptor agonists for inflammatory and neuropathic pain** *G.M. Dondio (Baranzate, Italy)*	
16.00-16.25	Main Lecture (ML60) **Specific kappa opioid receptor agonists** *G. Ronsisvalle (Catania, Italy)*	
16.30-18.00	**Poster Session B** **Exhibition**	Foyer
20.00-23.00	**Gala Dinner** (Villa Cicogna, San Lazzaro di Savena)	

Friday, September 22, 2000

9.00-9.45	Plenary Lecture (PL3) Chairman: *P. Andrews (Brisbane, Australia)* **The continuing evolution of the drug discovery process in the pharmaceutical industry** *E. Ratti (Verona, Italy)*	Europauditoriu
9.50-10.20	Coffee Break	
Section A	**Oral Communications** Chairman: *V. Tortorella (Bari, Italy)*	Sala Italia
10.25-10.40	OC13 **Discovery of the malonate Src SH2 binder RU85052. Synthesis and structure-activity studies** *P. Deprez (Romainville, France)*	
10.45-11.00	OC14 **Hydrogen bond activation of a Tyr-Arg-Tyr proton shuttle in the G protein-coupled β_1-adrenoceptor** *R.H. Davies (Cardiff, Wales, UK)*	
11.05-11.20	OC15 **Crystal structures of human farnesyl transferase protein and structure-aided approach for lead optimization** *A. Laoui (Vitry-sur-Seine, France)*	
Section B	**Oral Communications** Chairman: *P.L. Ornstein (Indianapolis, IN, USA)*	Europauditoriu
10.25-10.40	OC16 **Polymer-supported reagents as versatile tools in combinatorial chemistry and total synthesis** *J. Habermann (Cambridge, UK)*	
10.45-11.00	OC17 **CombiGrid, a computer program for the structure-based design of combinatorial libraries** *V. Tschinke (Basel, Switzerland)*	
11.05-11.20	OC18 **High throughput measurements and prediction of physico chemical parameters to predict absorption, an integrated approach** *C. Peake (Forest Row, East Sussex, UK)*	

Section C	**Oral Communications** Chairman: *E. Aiello (Palermo, Italy)*	Sala Topazio
10.25-10.40	OC19 **Synthesis and pharmacological properties of novel ascomycin derivatives modified in the binding domain** *K. Baumann (Vienna, Austria)*	
10.45-11.00	OC20 **Glucose-6-phosphatase catalytic enzyme inhibitors; synthesis and in vitro evaluation of novel 4,5,6,7-tetrahydrothienipyridines** *P. Madsen (Malov, Denmark)*	
11.05-11.20	OC21 **Synthetic approaches to heterocyclic conformationally constrained aminobutyrophenones as active agents on dopamine and serotonin receptors** *E. Raviña (Santiago de Compostela, Spain)*	
11.25-13.00	**Poster Session C**	Foyer
13.00-14.00	**Lunch Break**	

Friday, September 22, 2000

Theme 13	**Polyamines as Templates for Transmitter Receptor Ligands** Chairman: *P.N.R. Usherwood (Nottingham, UK)*	Sala Topazio
14.00-14.25	Main Lecture (ML61) **Multiple sites of action of polyamines on signalling proteins** *P.N.R. Usherwood (Nottingham, UK)*	
14.30-14.55	Main Lecture (ML62) **Analogues of polyamine alkaloids and their synthetic advantages** *M. Hesse (Zurich, Switzerland)*	
15.00-15.25	Coffee Break	
15.25-15.40	OC22 **Polyamine toxins - synthetic and mechanistic studies** *K. Stroemgaard (Copenhagen, Denmark)*	
15.45-16.00	OC23 **Selective antagonism of ionotropic receptors by philanthotoxin analogues** *I.A. Mellor (Nottingham, UK)*	
16.05-16.30	Main Lecture (ML63) **Highly negatively charged region identified in the vestibule of the nicotinic acetylcholine receptor's ion channel** *M.G. Bixel (Berlin, Germany)*	

Theme 14	**New Technologies** Chairman: *G. Giardina (Baranzate, Italy)*	Sala Italia
14.00-14.25	Main Lecture (ML64) **Bioinformatics and the data deluge in drug discovery** *C. Rawlings (Abingdon, UK)*	
14.30-14.55	Main Lecture (ML65) **Molecular diversity: how do we measure it? Has it lived up to its promise?** *Y.C. Martin (Abbott Park, IL, USA)*	
15.00-15.25	Coffee Break	
15.35-16.00	Main Lecture (ML66) **Technology platforms for combinatorial lead finding** *E. Felder (Nerviano, Italy)*	
16.05-16.30	Main Lecture (ML67) **NMR-screening: a paradigm shift for finding ligands for drug discovery** *M. Shapiro (Summit, NJ, USA)*	

Theme 15	**Pharmacokinetic Lead Optimisation** Chairman: *B. Testa (Lausanne, Switzerland)*	Europauditorium
14.00-14.25	Main Lecture (ML68) **Biological criteria in PK optimization** *J. Dressman (Frankfurt am Main, Germany)*	
14.30-14.55	Main Lecture (ML69) **Physicochemical properties in pharmacokinetic lead optimisation** *S.D. Kraemer (Zurich, Switzerland)*	
15.00-15.25	Coffee Break	
15.35-16.00	Main Lecture (ML70) **Structure–metabolism relations** *B. Testa (Lausanne, Switzerland)*	
16.05-16.30	Main Lecture (ML71) **Prediction of drug toxicity** *M. Cronin (Liverpool, UK)*	
16.35	**Closing** **Presentation of the XVII ISMC**	Europauditorium

POSTER SESSIONS

Session A: Tuesday, September 19

PA-001 **Bisphosphonate prodrugs: selective synthesis of mixed anhydride esters of clodronate**
M.J. Ahlmark, J.J. Vepsäläinen (Kuopio, Finland)

PA-002 **Conformational studies on synthetic peptides with prolactin-releasing activity in a membrane mimetic environment**
S. Albrizio, A. D'Ursi, D. Picone, P. Rovero, P.A. Temussi (Napoli, Italy)

PA-003 **Electrospray mass spectrometry study of dicationic [1$_4$]imidazoliophanes**
N. Mesquida, I. Dinarès, M. Vilaseca, *E Alcalde* (Barcelona, Spain)

PA-004 **Molecular modelling, synthesis and antitumour activity of carbocyclic lexitropsins with chlorambucil moieties**
D. Bartulewicz, K. Bielawski, A. Rózanski (Bialystok, Poland)

PA-005 **Computational simulations of recognition of new benzimidazole derivatives by the 5-HT$_4$R**
M.L. López-Rodríguez, *B. Benhamú*, A. Viso, M. Murcia, E. Álvaro, J. Sallés, L. Pardo (Madrid, Spain)

PA-006 **DNA-Binding properties and biological activity of novel aromatic amidines in cultured human skin fibroblasts**
K. Bielawski, A. Bielawska, J. Palka (Bialystok, Poland)

PA-007 **Binding models for inhibitors of the receptor tyrosine kinases PDGFR-β and FGFR-1**
A. Botzki, S. Dove (Regensburg, Germany)

PA-008 **Biologically active substituted 1,5-benzodiazepine-2-one**
V.I. Bozhanov, L.V. Dmitrikova, S.P. Ivonin (Dnepropetrovsk, Ukraine)

PA-009 **Novel substituted oxadiazepines with glucose lowering properties**
A.N. Bowler, J.P. Kilburn, S. Engelhardt, G.M. Danielsen, P. Kurtzhals (Måløv, Denmark)

PA-010 **Synthesis and biological evaluation of 3-alkylamino-7-chloro-4*H*-1,2,4-benzothiadiazine 1,1-dioxides as k_{ATP} channel openers structurally related to BPDZ 73**
S. Boverie, B. Becker, F. Somers, P. de Tullio, D. Dewalque, M.-H. Antoine, P. Arkhammar, F.E. Nielsen, J.B. Hansen, J. Damas, J. Delarge, P. Lebrun, B. Pirotte (Liège, Belgium)

PA-011 **Synthesis of nicotine derivatives using solid supported reagents**
G. Brusotti, S.V. Ley (Cambridge, UK)

PA-012 **Synthesis of new simplified analogs of artemisinin: insight to their mechanism of action**
B. Camuzat-Dedenis, O. Provot, J. Mayrargue, H. Moskowitz, J. Cazelles, A. Robert, B. Meunier, L. Cicéron, F. Gay (Châtenay-Malabry, France)

PA-013 **COMFA model for antichagasic nitrofurane and nitrothiophene derivatives. Docking analysis on trypanothione reductase**
V. Martinez-Merino, *H. Cerecetto* (Montevideo, Uruguay)

PA-014 **Design and synthesis of heterocycles containing conjugated polyhydroxybenzene derivatives as potential protein kinase inhibitors**
J.-W. Chern, P.-S. Hsu (Taipei, Taiwan)

PA-015 **Force field study of the interaction between dihydropyridine derivatives and a synthetic Ca^{2+} channel**
M. Cotta Ramusino, M.R. Varì (Roma, Italy)

PA-016 **7-Substituted 3-isopropylamino-4*H*-1,2,4-benzothiadiazine 1,1-dioxides as potent K_{ATP} channel openers: synthesis and biological *in vitro* evaluation**
P. de Tullio, F. Somers, J. Ouedraogo, S. Boverie, M.-H. Antoine, B. Becker, F.E. Nielsen, P. Arkhammar, J.B. Hansen, J. Delarge, P. Lebrun, B. Pirotte (Liège, Belgium)

PA-017 **SAR and rational design of SRC SH2 binders around a heterocyclic scaffold. Identification of RU84687, a subnanomolar and Src SH2 selective binder**
P. Deprez, E. Mandine, I. Baholet, C. Bardelay, R. Botham, P. Broto, J.P. Marquette, D. Massardier, E. Sarubbi, A. Vermond, E. Sarubbi, S. Viet, G. Lange, B. Schoot, D. Lesuisse (Romainville, France)

PA-018 ***In silico* studies for the screening and design of pharmacologycally active compounds**
E. Estrada, A. Peña, A. Montero, E. Molina, E. Uriarte, L. Santana (Santiago de Compostela, Spa

PA-019 **A fast datamining method using 2/3D fingerprints**
A. Feriani, A. Pozzan, G. Tedesco, A.M. Capelli (Verona, Italy)

PA-020 **Design of new HIV-1 protease inhibitors**
M. Romero, L. Gracia, J.J. Cuadrado, *M. Font*, J.J. Lasarte, I. Prieto, P. Sarobe, F. Borrás, N.B. Centeno (Pamplona, Spain)

PA-021 **Towards the design of new peptidomimetic agents active in autoimmune diseases. Pharmacophore models based on the features of a set of immunomodulating peptides interacting with class II HLA proteins**
L. Gracia, M. Romero, J.J. Cuadrado, *M. Font* (Pamplona, Spain)

PA-022 **A pharmacophore search for phosphodiesterase 4 selective inhibition**
P. Fossa, G. Menozzi, L. Mosti (Genova, Italy)

PA-023 **Protection against oxidative damage by prodrugs of iron chelator N,N'-bis(3,4,5-trimethoxybenzyl)ethylenediamine N,N'-diacetic acid (OR10141)**
J.-B. Galey, P. Tachon, J. Dumats (Aulnay sous bois, France)

PA-024 **Comparative molecular field analysis on non structural-related 5-HT$_3$ antagonists**
E. Galvez, I. Iriepa, A. Morreale, D.B. Boyd (Madrid, Spain)

PA-025 **Superimposition-based protocol as a tool for determing bioactive conformations. II. Application to GABA$_A$ receptor**
E. Galvez, I. Iriepa, A. Morreale, D.B. Boyd (Madrid, Spain)

PA-026 **Superimposition-based protocol as a tool for determing bioactive conformations. I. Application to glycinergic receptor (GLYR)**
E. Galvez, I. Iriepa, A. Morreale, D.B. Boyd (Madrid, Spain)

PA-027 **Structure-activity relationships of nitrofurans and nitrobenzofurans with trypanocidal activity**
H. Cerecetto, R. Di Maio, G. Seoane, *M. Gonzáles* (Montevideo, Uruguay)

PA-028 **Field-interaction-ligand-optimization (F.I.L.O.) in the development of 3D-QSAR models for the rational design of selective adenosine receptor ligands**
F. Melani, *P. Gratteri*, C. Bonaccini, M. Adamo, V. Colotta (Firenze, Italy)

PA-029 **Discovery of potent and selective inhibitors of human steroid 5α-reductase 1, as drugs for androgen-dependent skin disorders**
A. Guarna, E.G. Occhiato, F. Machetti, D. Scarpi, G. Danza, M. Serio (Firenze, Italy)

PA-030 **Synthesis, photochemistry and application of coumarinylmethyl-caged cyclic nucleotides**
V. Hagen, B. Wiesner, S. Frings, U.B. Kaupp, J. Bendig (Berlin, Germany)

PA-031 **Solid-phase intermolecular radical reactions: sulfonyl radical addition to isolated alkenes and alkynes**
D. Hamza, S.J. Caddick, S.N. Wadman (Brighton, UK)

PA-032 **An adapted nested polymerase chain reaction for detection of bcr-abl fusion mRNA in chronic myeloid leukemia**
J. Kocki, A. Dmoszynska, J. Wojcierowski (Lublin, Poland)

PA-033 **Modeling of κ-opioid receptor/agonists interactions using pharmacophore-based and docking simulations**
A. Lavecchia, G. Greco, E. Novellino, F. Vittorio, G. Ronsisvalle (Napoli, Italy)

PA-034 **Synthesis of 1-(3,4-dihydroxy-5-nitrophenyl)-2-phenyl-ethanone and derivatives as potent and selective inhibitors of catechol-*O*-methyltransferase (COMT).**
D. Learmonth, J. Benes, A. Vieira-Coelho, P. Soares-da-Silva (S. Mamede do Coronado, Portugal)

PA-035 **Design and synthesis of 5-HT_{1A} receptor agonists and antagonists by computational simulations**
M.L. López-Rodríguez, M.J. Morcillo, B. Vicente, B. Benhamú, J. Sallés, X. Deupi, L. Pardo (Madrid, Spain)

PA-036 **New glycosidase inhibitors suitable for purification of enzymes by affinity chromatography**
I. McCort, A. Duréault, J.C. Depezay, O. Berteau, R. Daniel (Paris, France)

PA-037 **Effective access to enantiopure 2,4-ethanothreonines**
U. Meyer, A.W. Frahm (Freiburg, Germany)

PA-038 **Optimisation and validation of DiR methodology for virtual screening**
I. Morize (Vitry-sur-Seine, France)

PA-039 **Computer-aided prediction of biological activity spectra of substances: complex evaluation of lead compounds**
V. Poroikov, D. Filimonov (Moscow, Russia)

PA-040 **Docking of aciclovir analogs: success and pitfalls**
P. Pospisil, L. Scapozza, G. Folkers (Zurich, Switzerland)

PA-041 **The structural and electronical factors that contribute affinity for the time-dependent inhibition of COX-2 by NSAIDs**
R. Pouplana, J.J. Lozano, A. Riera, J. Ruiz (Barcelona, Spain)

PA-042 **Molecular properties prediction of drugs on the basis of structural similarity and physicochemical parameters**
O.A. Raevsky (Chernogolovka, Russia)

PA-043 **Oxobenzopyran derivatives as thrombin inhibitors**
F. Bourdel, F. Lacan, C. Doucet, L. Pochet, A. Caflish, B. Masereel, B Pirotte, *M. Reboud-Ravaux* (Paris, France)

PA-044 **Studies on enzymes involved in pantothenate biosynthesis**
A. Saldanha, S. Westaway, A. Smith, C. Abell (Cambridge, UK)

PA-045 **Molecular graphics study of some morpholin derivatives as new receptors σ ligands**
C. Saturnino, A. Capasso, G. Barone, M. Buonerba, G. De Martino (Salerno, Italy)

PA-046 **Synthesis of sulfur containing heterocycles from thioamides for the screening of their biological activity**
Yu.M. Shafran, V.A. Bakuley, V.S. Mokrushin (Ekaterinburg, Russia)

PA-047 **Synthesis of novel ibuprofen derivatives designed to combine antioxidant, antiinflammatory and neuroprotective activity**
I.C. Siskou, E.A. Rekka, A.P. Kourounakis, D. Galanakis, P.N. Kouronakis (Thessaloniki, Greece)

PA-048 **Application of pharmacophore models in the development of atypical antipsychotics**
B.G. Tehan, E.J. Lloyd, M.G. Wong (Parkville, Australia)

PA-049 **Pharmacochemical study of the relationship between biological and oxidative stress**
K. Tsiakitzis, A.P. Kourounakis, Ek. Tani, P.N. Kourounakis (Thessaloniki, Greece)

PA-050 **Preparation and *in vitro* trypanocydal activity of (+)-euryfuran derivatives**
J.A. Valderrama, M. Cortés, D. Pessoa-Mahana, M. Preite, J. Benites, A. Rojas de Arias, H. Nakayama, S. Torres, A. Segovia, J. Miret (Santiago, Chile)

PA-051 **1,2,3,4-Tetrahydroisoquinoline- and indole-based ligands for the 5-HT_7 receptor. Synthesis and molecular modeling of ligands and the receptor**
E.S. Vermeulen, C.J. Grol, H.V. Wikström (Groningen, The Netherlands)

PA-052 **Natural system of organic compounds (NSOC) as a guide in molecular diversity**
O.N. Voskresensky (Odessa, Ukraine)

PA-053 **Synthesis and SAR study of novel 5-aryl benzimidazolinones as progesterone receptor antagonists**
P. Zhang, E.A. Terefenko, Z. Zhang, Y. Zhu, K. Marschke, D. Mais (Radnor, USA)

PA-054 **New N-3 substituted 2,3-benzodiazepines with AMPA antagonist activity**
J. Barkóczy, Z. Rátkai, G. Simig, G. Lévai, G. Szabó, G. Szénási (Budapest, Hungary)

PA-055 **8-Azaspiro[4.5]decane-7,9-dione derivatives as selective antagonists at the α_{1D} adrenergic receptor**
D. Barlocco, F. Montesano, G. Cignarella, G. Motta, E. Poggesi, A. Leonardi (Milano, Italy)

PA-056 **BMY 7378 analogs as selective antagonists at the α_{1D} adrenergic receptor**
D. Barlocco, F. Montesano, G. Cignarella, E. Poggesi, G. Motta, A. Leonardi (Milano, Italy)

PA-057 **Design and synthesis of new napthosultam and naphtholactam derivatives as 5-HT_7R ligands**
M.L. López-Rodríguez, M.J. Morcillo, E. Porras, *B. Benhamú*, L.J. Soto, J.A. Ramos, J.L. Lavandera (Madrid, Spain)

PA-058 **Philanthotoxin-343: a structure-activity study on the nicotinic acetylcholine receptor**
T. Brier, K. Stromgaard, I. Mellor, K. Andersen, J. Jaroszewski, P. Krogsgaard-Larsen, P. Usherwood (Nottingham, UK)

PA-059 **Inhibition of nicotinic and muscarinic acetylcholine receptors by polyamine amides**
R. Budriesi, A. Chiarini, S. Rizoli, T.J. Brier, I.R. Mellor, P.N.R. Usherwood, K. Popaj, M. Lochner, Y. Li, M. Hesse (Bologna, Italy)

PA-060 **Cardiovascular characterization of [1,4]thiazino[3,4-*c*][1,2,4]oxadiazol-1-one-derivatives: selective myocardial calcium channel modulators**
R. Budriesi, B. Cosimelli, P. Ioan, D. Spinelli, A. Chiarini (Bologna, Italy)

PA-061 **Pyrazolo-triazolo-pyrimidine derivatives as adenosine receptor ligands: a search for A_{2B} adenosine receptor antagonists**
B. Cacciari, G. Spalluto, P.G. Baraldi, R. Romagnoli, K. Varani, S. Gessi, S. Merighi, P.A. Borea (Ferrara, Italy)

PA-062 **Synthesis and evaluation of *trans*-2-amino-5(or 6)-chloro-6(or 5)-hydroxy-1-phenyl-2,3-dihydro-1*H*-indenes as dopamine receptor ligands**
A. Di Stefano, G. Luisi, *I. Cacciatore*, P. Sozio, B. Mosciatti, G.M. Cingolani, F. Pinnen (Chieti, Italy)

PA-063 **Synthesis and binding studies of 1'-*C*-methyl-2-chloroadenosine and its N^6-substituted derivatives as adenosine receptor agonists**
L. Cappellacci, P. Franchetti, S. Marchetti, B. Costa, C. Martini, M. Grifantini (Camerino, Italy)

PA-064 **4,5-Dihydro-2-phenyl-1,2,4-triazolo[1,5-a]quinoxaline derivatives as highly potent and selective A_3 adenosine receptor antagonists**
D. Catarzi, V. Colotta, F. Varano, L. Trincavelli (Firenze, Italy)

PA-065 **6-Aralkylamino-1,2-dihydro-2-phenyl-1,2,4-triazolo[4,3-a]quinoxalin-1-ones as A_{2A} adenosine receptor antagonists**
V. Colotta, D. Catarzi, F. Varano, L. Trincavelli (Firenze, Italy)

PA-066 **Benzosubstituted 2-phenyl-1,2,4-triazolo[4,3-a]quinoxalin-1-ones. Synthesis and binding activity on adenosine receptors**
V. Colotta, D. Catarzi, F. Varano, L. Trincavelli (Firenze, Italy)

PA-067 **Conversion of a weak HTS hit to a potent CCR2B (MCP-1) receptor antagonist**
D.G. Cooper, T.A. Berkhout, E.K. Dodds, I.T. Forbes, J. Gohil, P.H.E. Groot, D.M.B. Hickey, R.J. Ife, M.L. Meeson, K. Mooreş, M. Stockley (Harlow, UK)

PA-068 **3-Aryl-[1,2,4]triazino[4,3-a]benzimidazol-4(10H)-ones: selective A_1 adenosine receptor antagonists**
G. Primofiore, *F. Da Settimo*, S. Taliani, E. Novellino, G. Greco, A. Lavecchia, L. Trincavelli, C. Martini (Pisa, Italy)

PA-069 **Indol-3-ylglyoxylylamide derivatives probing the existence of a hydrogen acceptor/donor group in the S1 region of the benzodiazepine receptor binding site**
G. Primofiore, *F. Da Settimo*, S. Taliani, A.M. Marini, G. Greco, E. Novellino, L. Trincavelli, C. Martini (Pisa, Italy)

PA-070 **Conformational studies on a new synthetic MOG glycopeptide antigen able to block demyelinating autoantibodies in multiple sclerosis**
A.M. D'Ursi, A. Carotenuto, E. Nardi, E. Mastrangelo, A.M. Papini, F. Lolli, F. Pinto, P. Rovero (Salerno, Italy)

PA-071 **Met-Ile-Phe-Leu derivatives: full and partial agonists towards formyl peptide receptors of human neutrophils**
A. Dalpiaz, A. Scatturin, R. Pecoraro, P.A. Borea, K. Varani, S. Traniello, S. Spisani (Ferrara, Italy)

PA-072 **N-Ureido peptide derivatives as antagonists toward human neutrophil formyl peptide receptor**
A. Dalpiaz, S. Spisani, A. Scatturin, S. Bertuolo, M.E. Ferretti, S. Trainiello, G. Vertuani (Ferrara, Italy)

PA-073 **β_3-Adrenergic receptor ligands: synthesis of new derivatives and computational studies**
L. Kassi, *M. De Amici*, C. De Micheli, G. Carrea, G. Colombo, G. Ottolina (Milano, Italy)

PA-074 **Novel 2,4-diaminoquinazolines: synthesis and antagonist activity at α_1-adrenoceptors**
D. Giardinà, P. Angeli, M. Buccioni, U. Gulini, G. Marucci, C. Melchiorre, A. Leonardi, E. Poggesi (Camerino, Italy)

PA-075 **Novel N-substituted-N'-(9-benzyl-2-phenyl-8-azapurin-6-yl)urea derivatives as ligands for A_1 and A_3 adenosine receptors**
G. Biagi, *I. Giorgi*, O. Livi, F. Pacchini, V. Scartoni (Pisa, Italy)

PA-076 **Synthesis, chiral separation and pharmacology of highly potent histamine H_2 receptor agonists related to arpromidine**
C. Götte, J. Kracht, A. Meister, A. Schuster, S. Bollwein, F. Schalkhaußer, G. Bernhardt, A. Buschauer (Regensburg, Germany)

PA-077 **[Nphe^1]-NC(1-13)-NH_2, a novel selective ORL-1 receptor antagonist**
R. Guerrini, S. Salvadori, G. Calò, D. Regoli (Ferrara, Italy)

PA-078 **New cyclopentenopyridine derivatives. A potent, orally active, selective endothelin ET_A receptor antagonist**
T. Hayama, K. Niiyama, N. Ohtake, H. Takahashi, N. Kawanishi, T. Yoshizumi, H. Okada, T. Kano, M. Okada, Y. Ishii, M. Nishikibe (Ibaraki, Japan)

PA-079 **Rapid functional screening at P2Y and dopamine receptors by measuring intracellular calcium with a fluorescence microplate reader**
B. Höfgen, J.M. Quillan, J. Lehmann, M.U. Kassack (Bonn, Germany)

PA-080 **Ligands for the common allosteric site of acetylcholine M_2-receptors: optimization of the hexamethonium compounds**
U. Holzgrabe, W. Bender, R. Pick, M.H. Botero, E. Balatková, C. Tränkle, K. Mohr (Würzburg, Germany)

PA-081 **Argininamides with acceptor-substituted guanidino groups: potent neuropeptide Y Y_1 antagonists and putative prodrugs**
C. Hutzler, J. Kracht, E. Schreiber, G. Bernhardt, S. Dove, A. Buschauer (Regensburg, Germany)

PA-082 **Suramin and suramin analogues as inhibitors of G-protein coupled receptor kinase 2 (GRK2**
M.U. Kassack, P. Nickel, T. Haga, W. Sadée (Bonn, Germany)

PA-083 **Spiro[(1,3-diazacyclopent-1-ene)-5,2'-(5',6'-dimethylindane)]: a new α-adrenergic partial agonist. Two synthetic approaches**
J.-M. Lacoste, C. Courchay, J.-J. Descombes, T.J. Verbeuren, A. Cordi (Suresnes, France)

PA-084 **Chiral conformationally restricted analogues of lidocaine as ω_3 receptor ligands**
G. Lentini, F. Corbo, C. Franchini, G. Genchi, A. Scilimati, V. Tortorella (Bari, Italy)

PA-085 **Synthesis and pharmacology of a novel series of 11-substituted (*R*)-aporphines**
T. Linnanen, N. Mohell, G. Nordvall, L. Unelius, A.M. Johansson (Uppsala, Sweden)

PA-086 **Design and synthesis of new arachidonic acid derivatives as endocannabinoid uptake inhibitors**
M.L. López-Rodríguez, I. Lastres-Becker, A. Viso, S. Rodríguez, S. Ortega-Gutiérrez, J.J. Fernández-Ruiz, J.A. Ramos (Madrid, Spain)

PA-087 **Synthesis and biology of NBD-derivatives of NECA as new fluorescent probes for adenosine receptors**
M. Macchia, S. Bertini, V. Di Bussolo, M. Gesi, A. Lucacchini, C. Martini, F. Minutolo, F. Salvetti, D. Tuscano (Pisa, Italy)

PA-088 **Synthesis of (+) and (–)-*cis*-2-[(1-adamantylamino)-methyl]-1-phenylcyclopropane derivative as probes for σ_1 and σ_2 binding sites**
A. Marrazzo, O. Prezzavento, F. Vittorio, M.S. Pappalardo, G. Ronsisvalle (Catania, Italy)

PA-089 **Antimuscarinic activity of bicyclic dioxolanes**
M. Giannella, M. Pigini, *A. Piergentili*, W. Quaglia, S.K. Tayebati (Camerino, Italy)

PA-090 **1-Aryl-3-[1,5]naphthyridin-4-yl-ureas – the first selective orexin-1 receptor antagonists**
J. Arch, S. Brough, W. Chan, M. Duxon, M. Hadley, P. Jeffery, J. Jerman, A. Johns, D. Jones, A. Haynes, *R. Porter*, D. Smart, N. Upton (Harlow, UK)

PA-091 **PLE-based resolution of piperidine analogues of cocaine and biological activity of novel N-methyl-4-(diphenylmethoxy)-3-carbomethoxypiperidines**
M. Roberti, R. Rondanin, R. Baruchello, A. Mazzali, F.P. Invidiata, M. Rossi, D. Simoni (Bologna Italy)

PA-092 **Synthesis of hexahydropyrazino[2,1-c][1,4]benzoxazine derivatives as comformationally hindered analogues of N-(2-methoxyphenyl)piperazine-based α_1 adrenoceptor ligands**
G. Romeo, L. Materia, F. Russo, K.P. Minneman (Catania, Italy)

PA-093 **Synthesis and inhibitory activity towards human neutrophil elastase of some oximic and hydroxylaminic derivatives**
A. Rossello, A. Balsamo, F. Mamone, E. Orlandini, G. Cercignani (Pisa, Italy)

PA-094 **Agonist activity at the kinin B_1 receptor: structural requirements of the central tetrapeptide**
A. Di Fenza, S. Meini, L. Quartara, C.A. Maggi, F. Formaggio, C. Toniolo, *P. Rovero* (Salerno, Italy)

PA-095 **Synthesis of 1,2,4-oxadiazole-based peptidomimetics as potential GPIIb/III antagonists**
M. Sollner, P. Kolenc, P. Vitezic, M. Stegnar (Ljubljana, Slovenia)

PA-096 **Novel 1,3-dioxolanes as α_1-adrenergic antagonists**
C. Sorbi, M. Manicardi, R. Gallesi, P. Angeli, G. Marucci, M. Buccioni, L. Brasili (Modena, Italy)

PA-097 **Pyrazolo-triazolo-pyrimidine as human A_3 adenosine receptor antagonists: influence of the substituent at N^8 pyrazole nucleus**
G. Spalluto, P.G. Baraldi, B. Cacciari, R. Romagnoli, S. Moro, E. Leung, K. Varani, S. Gessi, S. Merighi, P.A. Borea (Trieste, Italy)

PA-098 **Quinolizidine derivatives as ligands for sigma receptors**
A. Sparatore, F. Novelli, F. Sparatore (Milano, Italy)

PA-099 **Spiro [3,4-dihydro-6/7-R-1,2,4-benzotriazino-3,4'-(1'-substituted)piperidines] and related compounds as ligands for sigma receptors**
F. Novelli, *F. Sparatore* (Genova, Italy)

PA-100 **Synthesis and pharmacological characterization of [^{3}H]-MRE 3008-F20: the first radioligand antagonist for the human A_3 adenosine receptors**
K. Varani, P.G. Baraldi, B. Cacciari, R. Romagnoli, S. Merighi, S. Gessi, P.A. Borea, E. Leung, G. Spalluto (Ferrara, Italy)

PA-101 **Tricyclic heteroaromatic system. 5,6-Dihydro-5-oxo-pyrazolo[1,5-c]quinazolines as excitatory amino acid antagonists**
F. Varano, D. Catarzi, V. Colotta, C. Costagli (Firenze, Italy)

PA-102 **Synthesis of a set of pyrazolo[1,5-c]quinazolines as novel glycine/NMDA antagonists**
F. Varano, D. Catarzi, V. Colotta, C. Costagli (Firenze, Italy)

PA-103 **The discovery of new antagonists of the adenosine A_{2B} receptor**
T.R. Webb, N. Melman, D. Lvovskiy, X. Ji, J. Linden, K.A. Jacobson (San Diego, USA)

PA-104 **Potential existence of the sequence of bovine leukemia virus cell receptor gene in human genome**
J. Wojcierowski, M. Gawlowicz, D. Koczkodaj, B. Marzec, A. Filip, T. Kubiatowski, J. Gawlowicz (Lublin, Poland)

PA-105 **Molecular models of receptor-ligand interactions for analysis of dynamics of pharmacological effects in vivo**
O.V. Zhuk, V.G. Zinkovsky, N.Ya. Golovenko, G.A Tokar, E.A. Stankevich, M.S. Zhuk (Odessa, Ukraine)

PA-106 **Isodynamic analysis of the minimal effective doses of the exogenic ligands of $GABA_A$-receptor complex as a method for the estimation of the mechanisms of their interaction with the CNS mediator system**
V.G. Zinkovsky, *O.V. Zhuk*, N.Ya. Golovenko, S.A. Silantiev, A.V. Sliskiy (Odessa, Ukraine)

PA-107 **Synthesis and pharmacological investigation of some novel 1,2- disubstituted–*s*-[1,2,4] triazolo quinazolones as antihypertensive agents**
V. Alagarsamy, U.S. Pathak (Sivakasi, India)

PA-108 **Discovery and structure-activity relationships of novel thrombin receptor antagonists**
J.C. Barrow, H.G.Selnick, P.G. Nantermet, T.N. Connolly, M.B. Young, K.R. Rittle, G.F. Lundel J.L. Pellicore, K.L. Glass, P.L. Ngo, J.J. Hutchinson, M.J. Breslin, C. Condra, J. Karczewski, A. Stern, R.M. Freidinger, R. Gould (West Point, USA)

PA-109 **Synthesis of 2-lupinylindoles and 2-phenyl-3-lupinylindoles as platelet anti-aggregating compounds**
L. Mina, A. Bennicelli, *V. Boido*, F. Sparatore, F (Genova, Italy)

PA-110 **Studies on new basic NO-donor 1,4-dihydropiridines**
D. Boschi, G. Caron, C. Cena, S. Visentin, A. Di Stilo, R. Fruttero, A. Gasco (Torino, Italy)

PA-111 **Pharmacological characterization of new antiplatelet benzopyrano[4,3-d]pyrimidines**
E. Barocelli, V. Ballabeni, M. Tognolini, M. Chiavarini, S. Bertoni, *O. Bruno* (Genova, Italy)

PA-112 **New antithrombotic agents: benzothiophene derivatives as inhibitors of the tPa/PAI-1 complex formation**
G. De Nanteuil, C. Lila, A. Rupin, T.J. Verbeuren (Suresnes, France)

PA-113 **Protection of isolated perfused rat heart against ischemia-reperfusion evoked injury by glutapyrone**
J. Briede, A. Velena, E. Bisenieks, *G. Duburs*, J. Uldrikis, J. Poikans (Riga, Latvia)

PA-114 **The design and synthesis of novel ventricular defibrillating agents**
M. Erez, O. Levy, D. Varon, E. Keinan (Haifa, Israel)

PA-115 **Vitamin C and E analogs: design, synthesis, antioxidant activity and protection against ischemia-reperfusion injuries**
S. Manfredini, S. Vertuani, *D. Govoni*, B. Manfredi, G. Rossoni, G. Calviello, P. Palozza (Ferrara, Italy)

PA-116 **New pyrimidine or pyran fused derivatives with inhibitory activity on human platelet aggregation**
G.C. Grossi, M. Di Braccio, G. Roma, G. Leoncini, M.G. Signorello (Genova, Italy)

PA-117 **Effects of SUN C5174, a novel 5-HT_2 receptor antagonist, on various experimental models of peripheral circulatory disorder**
N. Inomata, A. Ogata, C. Takiguchi, H. Takagi, Y. Kamiide, Y. Horikawa, Y. Hayashi, A. Yamaki A. Mizuno (Gunma-ken, Japan)

PA-118 **Synthesis and serotonin 2 receptor antagonist activity of 5-aminoalkyl-substituted pyrrolo[3,2-*c*]azepines and related compounds**
A. Mizuno, T. Kamei, M. Shibata, N. Inomata, A. Ogata, C. Takiguchi, T. Shimamoto, K. Nakanishi, Y. Hayashi (Osaka, Japan)

PA-119 **Dihydropyridazinone derivatives as novel antihypertensive agents**
A.-R. Lee, S.-T. Tang, M.-H. Yen (Taipei, Taiwan)

PA-120 **4-Nitropyrazole derivatives as new exogenic donors of nitric oxide**
V. Makarov, N. Grigoriev, M. Schmidtke, V.A. Parshin, V. Granik (Moscow, Russia)

PA-121 **Design & synthesis of selective PDE5 inhibitors for the treatment of MED**
S.A. Ballard, K.C. Beaumont, M.E. Bunnage, *J.P. Mathias*, S.D.A. Street, A. Wood (Sandwich, UK)

PA-122 **Secosteroids as cardenolide analogues**
L.G. Sevillano, F. Tomé, E. Caballero, *M. Medarde*, A. San Feliciano (Salamanca, Spain)

PA-123 **Peptide to synthetic thrombin inhibitor by pharmacophore based design of a novel series of 4-aminopyridines**
S.A.M. Mérette, P. Greenidge, C.A. Goodwin, M.F. Scully, J.J. Deadman

PA-124 **Synthesis of 2-oxopyridine, 2,5-dioxopyridine and 2,5-dioxoindenopyridine derivatives as potential cardiotonic agents**
L. Mosti, G.Menozzi, P. Fossa, S. Schenone (Genova, Italy)

PA-125 **Synthesis and biological activities of the 2-piperazinone derivative (M55190), an orally active and highly specific factor Xa inhibitor**
H. Nishida, Y. Miyazaki, T. Mukaihira, F. Saitoh, K. Harada, H. Shimada, N. Mizuno, T. Matsusue, A. Okamoto, Y. Hosaka, M. Matsumoto, M. Kamiya, M. Kurokawa, K. Mizuguchi, S. Ohnishi, H. Mochizuki (Shizuoka, Japan)

PA-126 **Novel thrombin inhibitors with azaphenylalanine scaffold**
A. Obreza, A. Zega, U. Urleb (Ljubljana, Slovenia)

PA-127 **The discovery of DPC 423, a highly potent, selective and orally bioavailable inhibitor of blood coagulation factor Xa**
D.J. Pinto, M.J. Orwat, S. Wang, J.R. Pruitt, J.M. Fevig, M.L. Quan, Q. Han, E. Amparo, J. Cacciola, L.L. Bostrom, R. Knabb, J.M. Luettgen, M.R. Wright, B.J. Aungst, P.C. Wong, P.Y.S. Lam, R.R. Wexler (Wilmington, USA)

PA-128 **Di-substituted imidazoles as inhibitors of neuronal nitric oxide synthase**
L. Salerno, V. Sorrenti, F. Guerrera, M.A. Siracusa, C. Di Giacomo, A. Vanella (Catania, Italy)

PA-129 **N-1 Substituted pyrimidin-4-ones: novel, orally active inhibitors of lipoprotein associated phospholipase A_2**
S.A. Smith, H.F. Boyd, S.C.M. Fell, S.T. Flynn, D.M.B. Hickey, R.J. Ife, C.A. Leach, C.H. Macphee, K.J. Milliner, K.E. Moores, I.L. Pinto, R. Porter, D.A. Rawlings, I.G. Stanfield, D.G. Tew, C.J. Theobald, C.M. Whittaker (Harlow, UK)

PA-130 **The identification of a potent, water soluble inhibitor of lipoprotein associated phospholipase A_2**
S.A. Smith, H.F. Boyd, D.M.B. Hickey, R.J. Ife, C.A. Leach, C.H. Macphee, K.J. Milliner, I.G. Stansfield, C.J. Theobald (Harlow, UK)

PA-131 **New arylpiperazine derivatives as antagonists of the human cloned 5-HT_4 receptor isoforms**
J.L. Soulier, S. Curtet, I. Zahradnik, M. Giner, I. Berque-Bestel, J. Mialet, F. Lezoualc'h, S. Sicsic, R. Fischmeister, M. Langlois (Châtenay-Malabry, France)

PA-132 **The discovery of pseudopeptide antagonists of the atrial natriuretic peptide clearance receptor (Part 1)**
C.L. Dantzman, C.A. Veale, P.D. Edwards, R.T. Jacobs, M. Murphy, R.C. Mauger, K.K Pine, W.E. Palmer, G.B. Steelman, M. Sylvester, V. Alford, E.P. Vacek, S.T. Dock, T.W. Davenport, G.A. Hostetler, D. Aharony, R.A. Bialecki, W.L. Rumsey (Wilmington, USA)

PA-133 **The discovery of pseudopeptide antagonists of the atrial natriuretic peptide clearance receptor (Part 2)**
C.A. Veale, P.D. Edwards, R.T. Jacobs, C.L. Dantzman, M. Murphy, R.C. Mauger, K.K. Pine, W.E. Palmer, G.B. Steelman, M. Sylvester, V. Alford, E.P. Vacek, S.T. Dock, T.W. Davenport, G.A. Hostetler, D. Aharony, R.A. Bialecki, W.L. Rumsey (Wilmington, USA)

PA-134 **4-Aryl-7,7,-dimethyl-4,6,7,8-tetrahydro-(1H,3H)-quinazoline-2,5-diones: synthesis, enantiomeric separation and pharmacological activity**
M. Yarim, S. Saraç, M. Ertan, F.S. Kiliç, K. Erol (Ankara, Turkey)

PA-135 **"Consol" solution for heart preservation**
S.Y. Berdyaev, *I.L. Zhidkov*, A.S. Ivanov, V.A. Kozhevnikov, I.I. Dementeva, G.F. Sheremeteva, V.I. Gretskaya, A.A. Philantencov (Moscow, Russia)

PA-136 **Oxygen consumption and lipolysis on white adipocytes induced by new NPY receptor antagonists**
I. Aldana, M. Aguado, J. Margareto, A. Martí, C. Frigola, B. Muro, A. Monge, J.A. Martínez (Pamplona, Spain)

PA-137 **Optically active 2-substituted carboxylic acids isosters of fibrates by 2-bromo esters**
A. Ammazzalorso, *R. Amoroso*, G. Bettoni, B. De Filippis (Chieti, Italy)

PA-138 **New 1,4-oxazine derivatives as nitric oxide donors with hypolipidemic and antioxidant properties**
M.C. Chrysselis, I.C. Siskou, E.A. Rekka, P.N. Kourounakis (Thessaloniki, Greece)

PA-139 **A new series of 3-alkylamino-5,6-diphenylpyridazines as ACAT inhibitors**
V. Dal Piaz, M.P. Giovannoni, D. Barlocco, B.M. Kwon, M.K. Kim, Y.K. Kim (Firenze, Italy)

PA-140 **Effect of cerebrocrast on the lipid metabolism in the STZ-DOCA diabetic rats**
J. Briede, *G. Duburs* (Riga, Latvia)

PA-141 **Design, synthesis and development of selective serotonin agonists for the treatment of obesity**
L.M. Harris, I.T. Crosby (Victoria, Australia)

PA-142 **Structure-activity relationship of a novel chemical family of MTP inhibitors with lipid-lowering properties**
J. Heeres, *L. Meerpoel*, L. Backx, R. Hendricks, P. Luyts, L. Van Der Eycken, L. Van Der Veken, B. Vergouwen, P. Roevens, D. De Chaffoy de Courcelles (Beerse, Belgium)

PA-143 **A new HMG-CoA reductase inhibitor, NK-104: QSAR studies**
M. Mutsukado, M. Suzuki (Funabashi, Japan)

PA-144 **Synthesis of a new series of aminophosphonate compounds with lipoprotein(a) lowering activity**
L.M. Nguyen, H.T. Phan, V.V. Diep, R. Azoulay, S. Florey, E. Niesor, C.L. Bentzen, M.O. Montjovent, R.J. Ife, S.E. Clarke (Geneva, Switzerland)

PA-145 **New chiral 3-amino-2-propanols as simple, potent inhibitors of cholesteryl ester transfer protein**
J.A. Sikorski, R.C. Durley, M.L. Grapperhaus, M.A. Massa, D.A. Mischke, B.L. Parnas, Y.M. Fobian, D.D. Honda, M. Zeng, B.R. McKinnis, D.T. Connolly, D.A. Heuvelman, B.J. Witherbee, K.C. Glenn, E.S. Krul, N.R. Rath, M.E. Smith (St. Louis, USA)

PA-146 **Synthesis of organosilicon heteroaromatic sulfides as cholesterol level lowering agents**
M. Veveris, K. Rubina, R. Abele, E. Abele, P. Arsenyan, I. Sleiksa, E. Lukevics (Riga, Latvia)

PA-147 **Synthesis and antiosteoporotic activity of new isoflavone derivatives**
E. Armani, G. Amari, M. Delcanale, E. Galbiati, M. Civelli, M. Giossi, P. Caruso (Parma, Italy)

PA-148 **Synthesis of new bioactive compounds on the basis of betulonic acid**
L. Baltina, O. Flekhter, L. Nigmatullina, F. Galin, O.A. Plyasunova, G. Tolstikov (Ufa, Russia)

PA-149 **Transformations of glycyrrhizic acid in relation to the biological activities**
L. Baltina, A.G. Pokrovskyi, G. Tolstikov (Ufa, Russia)

PA-150 **Effects of furocoumarins from the fruits of cow parsnip (*Heracleum* L. species) on the human leukemic cells**
A. Bogucka-Kocka, J. Kocki, T. Krzaczek (Lublin, Poland)

Session A: Tuesday, September 19

PA-151 **Consituents of euphorbiaceae: isolation and structure elucidation of a digalactosyl-diacyglycerol from *Euphorbia peplis* L.**
F. Cateni, J. Zilic, G. Falsone, E. Vitrotti (Trieste, Italy)

PA-152 **Synthesis of N-(N-benzoyl-S*-phenylalaninyl)-S*-phenylalaninol benzoate, isolated from *Zeyhera digitalis* roots**
M. Faccione, D. Ferreira Trevisan (Londrina, Brazil)

PA-153 **Development of betulinic and quinopimaric acids as a route to new drugs**
O. Flekhter, L. Nigmatullina, N. Medvedeva, E. Tret'yakova, O. Ashavina, G. Tolstikov (Ufa, Russia)

PA-154 **New molecules, new ideas; taurine and analogues in treatment strategies of 21st century diseases; an overview**
R.C. Gupta (Medziphema, India)

PA-155 **Derivatives of the natural product SB-219383 and synthetic analogues: potent inhibitors of bacterial tyrosyl tRNA synthetase**
D.W. Hamprecht, J.M. Berge, R.C.B. Copley, D.S. Eggleston, C.S.V. Houge-Frydrych, R.L. Jarvest, L.M. Mensah, P.J. O'Hanlon, A.J. Pope, S. Rittenhouse (Harlow, UK)

PA-156 **Isolation from *Barbarea verna* seeds and characterization of 2-phenylethyl glucosinolate, precursor of the potential chemoprotective phenethyl isothiocyanate**
J. Barillari, *R. Iori*, L. Lazzeri, D. Gueyrard, P. Rollin (Bologna, Italy)

PA-157 **Studies on aromatic compounds from *Tagetes lucida***
A. Maioli, C. Saturnino, G. De Martino, F. De Simone, L. Rastrelli, R. Aquino (Salerno, Italy)

PA-158 **Synthesis and biological activities of novel pyrimidine derivatives of 4,5-didehydro-5,6-dideoxy-*L*-ascorbic acid**
S. Raic-Malic, D. Svedruzic, T. Gazivoda, A. Nagl, A. Hergold-Brundic, J. Balzarini, E. De Clercq, *M. Mintas* (Zagreb, Croatia)

PA-159 **Cytotoxic and anti-proliferative effects of prenylated flavones from *Artocarpus elasticus***
M.S.J. Nascimento, H. Cidade, M.M. Pinto, M. Pedro, F. Cerqueira, A. Kijjoa (Porto, Portugal)

PA-160 **Rational approach in designing, synthesize and biologiacal evaluation of new flavonoid analogues as potential p56^{lck} protein tyrosine kinase inhibitors**
Z. Nikolovska-Coleska, Lj. Suturkova, K. Dorevski, T. Solmajer (Skopje, Republic of Macedonia)

PA-161 **Studies toward total synthesis of neocarzinostatin chromophore**
M.G. Soscia, S.J. Caddick (Brighton, UK)

PA-162 **An investigation on the antioxidant activity of Heracleum persicum**
E. Souri, P. Sarkhail (Teheran, Iran)

PA-163 **Albocycline and related derivatives produced by *Streptomyces sp* using liquid brewery waste as culture-medium**
A. Taddei, C. Castelli (Caracas, Venezuela)

PA-164 **The action of two sulfur containing carbamates against sulphate reducing bacteria**
F. Norberto, M.E.M. Araújo, S. Santos, M. Meireles, C. Mendes, A.R. Lino (Lisboa, Portugal)

Session B: Thursday, September 21

PB-001 **Synthesis of 4,5-dihydro-3-(3-pyridinyl)-5-isoxazolecarboxamide derivatives: new potent inhibitors of T-cell blast formation**
E.J. Freyne, *J.I. Andrés*, F. Deroose, J. Fernández, D. Petit, J.M. Alonso, G. Boeckx, R. Alvarez, W. Embrechts, J.M. Cid, E. Coesemans, A. Del Cerro, L.M. Font, A. Fontana, L. Iturrino, E. Matesanz, M. Cools, A. Megens, J. Van Wauwe (Toledo, Spain)

PB-002 **Synthesis and prostaglandin synthase inhibitory activity of new aromatic O-alkyloxime ethers substituted with methylsulfonamidic and methylsulfonyl groups on their aliphatic portion**
A. Balsamo, E. Orlandini, S. Rapposelli, M. Pinza, C. Milanese, F. Mancini (Pisa, Italy)

PB-003 **'Olomoucine' like compounds as inhibitors of c-Src for the prevention and treatment of osteoporosis**
R. Beerli, L. Widler, T. Buhl, P. Furet, R. Gamse, M. Kneissel, M. Susa, R. Wolf, J. Green, M Missbach (Basel, Switzerland)

PB-004 **2-Carboxy-tetrahydroquinoline derivatives: a novel class of glycine antagonists as potent antihyperalgesic agents**
B. Bertani, G. Alvaro, R. Di Fabio, D. Donati, S. Giacobbe, M. Quartaroli (Verona, Italy)

PB-005 **New prodrugs from the class of antiinflammatory non-steroidic acids**
Gh. Bora, L. Beu, E. Cotora, M. Bora, M. Ruta, V. Bora (Cluji-Napoca, Romania)

PB-006 **Spectroscopic studies of some copper (II) complexes with antiinflammatory drugs**
M. Bora, O. Cozar, I. Bratu, Gh. Bora, V. Bora (Cluji-Napoca, Romania)

PB-007 **A novel class of potent exceptionally selective, nonpeptidic δ opioid receptor agonists**
W. Brown, Z.-Y. Wei, B. Takasaki, N. Plobeck, D. Delorme, F. Zhou, H. Young, P. Jones, L. Gawell, R. Schmidt, S.-Y. Yue, C. Walpole, K. Payza, S. St-Onge, M. Labarre, C. Godbout, A. Jakob, J. Butterworth, A. Kammassah, J. Ducharme, P-E. Morin, D. Projean, T.-M. Tu, E. Roberts (Quebec, Canada)

PB-008 **Synthesis and biological activity of new potential PDE4 inhibitors**
O. Bruno, N. Arduino, S. Schenone, A. Ranise, F. Bondavalli (Genova, Italy)

PB-009 **Synthesis of plurisubstituted δ-lactones with antiinflammatory activity**
F. Cateni, G. Falsone, M.M. De Nardo (Trieste, Italy)

PB-010 **Diphenyl-cycloalkylenepyrazoles, a new class of inhibitors of cyclooxygenase-2**
N. Cazzolla, I. Coletta, M. Tomaselli, C. Marani Toro, M. Mabilia, M. Giannangeli, M. Brufani, M. Pinza (Pomezia, Italy)

PB-011 **5-Imidazol-1-yl-1H-benzimidazoles as dual IL-1/TNFα inhibitors: a central approach in the treatment of osteoarthritis**
B. Portevin, *G. De Nanteuil*, A. Fradin, J. Bonnet (Suresnes, France)

PB-012 **Substituted 4-(2,2-diphenylethyl)pyridine-N-oxides as phosphodiesterase-4 inhibitors: SAR study directed toward the improvement of pharmacokinetic parameters**
Y. Ducharme, M. Blouin, C. Brideau, C. Chan, N. Chauret, R. Frenette, R.W. Friesen, Y. Girard, P. Hamel, Z. Huang, T. Jones, F. Laliberte, C. Li, P. Masson, M. McAuliffe, D. Nicoll-Griffith, J. Silva, J. Yergey, R.N. Young (Quebec, Canada)

PB-013 **Design and synthesis of potent cyclic pseudopeptide human NK-2 antagonists**
D. Giannotti, M. Altamura, F. Canfarini, C. Di Bugno, A. Giolitti, S. Giuliani, A. Guidi, N.J.S. Harmat, R. Nannicini, F. Pasqui, R. Patacchini, E. Perrotta, A.R. Renzetti, C.A. Maggi (Firenze, Italy)

PB-014 **Phenyl substituted analogs of CDP-840 as phosphodiesterase-4 inhibitors with improved potency, oral activity and metabolic stability**
Y. Girard, M. Blouin, C. Brideau, C. Chan, N. Chauret, Y. Ducharme, M. Girard, D. Guay, P. Hamel, Z. Huang, D. Nicoll-Griffith, T. Jones, F. Laliberte, C. Li, M. Mc Auliffe, J. Silva, J. Yergei, R.N. Young (Quebec, Canada)

PB-015 **Novel fentanyl like analgesics**
C. Cano, *P. Goya*, N. Jagerovic, R. Giron, C. Goicoechea, M.I. Martín (Madrid, Spain)

PB-016 **Synthesis and inhibition of endotoxin-stimulated proinflammatory cytokines of substituted 2-amino-3-[1,3,4-oxadiazol-5-yl]-pyridines**
A. Hetzheim, D. Albrecht, S. Witt, C. Schütt (Greifswald, Germany)

PB-017 **AWD 12-343, a new orally active PDE 4 inhibitor. Synthesis and comparison with SB 207499, rolipram and AWD 12-281**
N. Höfgen, U. Egerland, H. Poppe, S. Küsters, T. Kronbach, S. Szelenyi (Radebeul, Germany)

PB-018 **Solid phase synthesis of 8-substituted 1,3,8-triazaspiro[4.5]decanones acting as nociceptin receptor ligands**
R. Hohlweg, C. Thomsen, I. Pettersson, R. Nielsen (Måløv, Denmark)

PB-019 **Discovery of potent and selective small molecule ORL1 receptor antagonist J-113397**
Y. Iwasawa, H. Kawamoto, S. Ozaki, Y. Itoh, M. Miyaji, S. Arai, H. Nakashima, T. Katoh, H. Ohta (Ibaraki, Japan)

PB-020 **Potent and orally active COX-2 inhibitors**
Y. Leblanc, S. Boyce, C. Brideau, C. Chan, N. Chauret, D. Claveau, R. Gordon, D. Nicoll-Griffith, S. Charleson, D. Ethier, A. Ford-Hutchinson, M. Gresser, E. Grimm, C.S. Li, D. Riendeau, I. Rodger, P. Roy, D. Visco, Z. Wang, E. Wong, R.N. Young, L. Xu, R. Zamboni, P. Prasit (Pointe Claire – Dorval, Quebec, Canada)

PB-021 **The synthesis of peptides with affinity to opioid and neuropeptide FF receptors**
A.W. Lipkowski, A. Misicka, I. Maszczynska, M. Lachwa, D.B. Carr, M. Yoshikawa, G. Toth (Warsaw, Poland)

PB-022 **Oxidized cyclodextrine as multipharmacophore carrier**
E. Marczak, A. Misicka, M. Lachwa, A.W. Lipkowski (Warsaw, Poland)

PB-023 **New potential opioid analgesics of the 1,3-substituted urea structure**
D. Matosiuk, S. Fidecka, L. Antkiewicz-Michaluk (Lublin, Poland)

PB-024 **Pharmacological evaluation of 4-substituted 1,5-diarylpyrazoles, analogues of celecoxib**
G. Menozzi, L. Mosti, L. Merello (Genova, Italy)

PB-025 **N-acyloxymethyl-2-azetidinones as human leukocyte elastase inhibitors**
A.B. Santana, E. Valente, J. Neres, *R. Moreira*, N. Palma, A.P. Grancho, A. Domingos, A. Clemente, J. Iley (Lisboa, Portugal)

PB-026 **Anti-inflammatory effect of thiazolyl and benzothiazolyl Schiff bases on pig cartilage**
A.M. Panico, V. Cardile, A.A. Geronikaki, B. Gentile, D. Urso (Catania, Italy)

PB-027 **A new series of polycondensed heterocyclic compounds, as potential anti-inflammatory**
A.M. Panico, V. Cardile, A. Santagati, S. Buccheri, F. Garufi (Catania, Italy)

PB-028 **The effect of new CCK-4 analogue on morphine-induced analgesia in rat tail flick test**
T. Proskuryakova, N. Pankratova, O. Petrichenko, V. Shokhonova (Moscow, Russia)

PB-029 **The synthesis of N-[substituted phenyl(pyridyl)carbonyl(sulfonyl)amino]1,2,3,6-tetrahydropyridines as potential antiinflammatory agents**
K.K. Redda, K.J. Yoon, T.L. Wilson, U.C. Onubogu, S. Williams (Tallahassee, USA)

PC-030 **Novel derivatives of tolfenamic acid as improved anti-inflammatory agents**
G. Ziakas, *E.A. Rekka*, A. Gavalas, P.N. Kourounakis (Thessaloniki, Greece)

PB-031 **Synthesis and antiinflammatory activities of some thiosemicarbazides, 1,3,4-oxadiazoles, 1,3,4-thiadiazoles and 1,2,4-triazole-3-thiones**
P. Erhan, *S. Gülay*, K. Pelin (Ankara, Turkey)

PB-032 **Synthesis and spasmolytic activity of 2-substituted thienopyrimidin-4-one derivatives**
N.A. Santagati, O. Prezzavento, G. Ronsisvalle, S. Spampinato (Catania, Italy)

PB-033 **Discovery of new lead inhibitors of aldose reductase from docking and structure-based dru design**
A.M. Ferrari, L. Costantino, *G. Rastelli* (Modena, Italy)

PB-034 **Evaluation of analgesic and anti-inflammatory activity of novel ß-lactam monocyclic compounds**
C. Saturnino, B.M. Fusco, M. Buonerba, G. Barone, F. Rocco, G. De Martino (Salerno, Italy)

PB-035 **Development of C5a agonists and antagonists**
R. Sbaglia, D.R. March, L. Proctor, S.M. Taylor, D.P. Fairlie (Queensland, Australia)

PB-036 **Synthesis and biological evaluation of new glycosidase inhibitors**
A. Spadaro, E. Bousquet, F. Vittorio, G. Ronsisvalle (Catania, Italy)

PB-037 **COX-2 inhibitors: pyrazolobenzothiazines as conformationally restricted 1,5-diarylpyrazole derivatives**
O. Tabarrini, V. Cecchetti, S. Sabatini, A. Fravolini (Perugia, Italy)

PB-038 **Synthesis, stereochemical features and prostaglandin biosynthesis inhibition of new 2,6-bis(1,1-dimethylethyl)phenol derivatives**
A. Tait, F. Vezzalini, G. Cannazza, D. Braghiroli, M. Baraldi, C. Parenti (Modena, Italy)

PB-039 **In-vitro test system for the evaluation of cyclooxygenase-1 (COX-1) and cyclooxygenase-2 (COX-2) inhibitors using bovine aortic coronary endothelial cells (BAEC) by a single high-performance liquid chromatography run with PDA-UV-detection**
G. Dannhardt, *H. Ulbrich* (Mainz, Germany)

PB-040 **Analgesic properties of benzoisothiazole/benzimidazole derivatives with acidic groups**
P. Vicini, L. Amoretti, C.A. Maggiali, V. Ballabeni, M. Tognolini, M. Chiavarini, F. Calcina, E Baroncelli (Parma, Italy)

PB-041 **New diarylmethylpiperazines as selective nonpeptidic δ opioid receptor agonists with improved binding affinity, agonist potency and *in vitro* metabolic stability**
C. Walpole, N. Plobeck, P. Schwarz, D. Delorme, S.-Y. Yue, W. Brown, K. Payza, S. St-Onge, M. Labarre, A. Kamassah, J. Ducharme, P.-E. Morin, D. Projean, E. Roberts (Montreal, Canada)

PB-042 **Toward new 6/7-substituted tropane analogues: synthesis, identification and *in vitro* studies**
A.J. Airaksinen, J. Vepsäläinen, A. Shvetsov, K. Bergström, S. Lötjönen, L. Tuomisto, P. Männistö, J. Hiltunen (Kuopio, Finland)

PB-043 **2-(1*H*-Imidazol-4-yl)-cyclopropyl carbamates: new histamine H_3 receptor antagonists: synthesis and structure-activity relationship studies**
S.M. Ali, Y. Rong, C.E. Tedford, S.L. Yates, G. Pawlowski, J. Jiang, K.R. Brunden (Cleveland, USA)

PB-044 **Identification and synthesis of the major metabolite of antiepileptic 10,11-dihydro-10-hydroxyimino-5H-dibenz[*b,f*]azepine-5-carboxamide**
A. Beliaev, J. Benes, D. Hainzl, A. Parada, M.J. Bonifácio, P. Soares-da-Silva (S. Mamede do Coronado, Portugal)

PB-045 **High-affinity σ_2 ligands: synthesis and SAFIR of *N*-cyclohexylpiperazine derivatives**
F. Berardi, S. Ferorelli, C. Abate, N.A. Colabufo, R. Calò, R. Perrone, V. Tortorella (Bari, Italy)

PB-046 **Synthesis of new dopaminergic alkyl- and arylthioapomorphines**
S. Berényi, S. Gyulai, G. Rusznyák (Debrecen, Hungary)

PB-047 **Synthesis of 1-methyl-5-(pyrazol-3- and –5-yl and 1,2,4-triazol-3- and 5-yl) 1,2,3,6-tetrahydropyridine derivatives and their evaluation as muscarinic receptor ligands**
A. Borioni, M.R. Del Giudice, C. Mustazza, F. Gatta, S.K. Tayebati, D. Vitali, F. Amenta (Roma Italy)

PB-048 **New derivatives of a promising serotoninergic compound**
D. Bózsing, G. Lax Koványi, S.I. Rátzné, G. Németh, L. Poszávácz, G. Simig, G. Lévay, I. Gacsályi, É. Schmidt (Budapest, Hungary)

PB-049 **Synthesis of 2,4-dihydro-1,2,4-benzothiadiazine 1,1-dioxide derivatives as potential allosteric modulators of AMPA receptors**
D. Braghiroli, G. Cannazza, A. Tait, F. Vezzalini, C. Parenti, G. Puia, M. Baraldi (Chieti, Italy)

PB-050 **Pyrazolo[1,5-a]pyrimidines: new peripheral benzodiazepine receptor ligands**
F. Bruni, S. Selleri, C. Costagli, A. Costanzo, G. Ciciani, G. Guerrini, P. Gratteri, B. Costa, C. Martini (Firenze, Italy)

PB-051 **(+)-ST1460: a potent atypical antipsychotic lead. Synthesis, further structure-activity relationships and biological studies**
S. Butini, G. Campiani, V. Nacci, E. Morelli, A. Cagnotto, M. Goegan, T. Mennini, P. Minetti, D. Mastroianni, N. Scafetta, B. Galletti, A. Di Cesare, M.A. Stasi, M. Castorina, O. Ghirardi, O. Tinti (Siena, Italy)

PB-052 **Synthesis of a novel TRH-related sulphonamido peptide**
L. Brunetti, *I. Cacciatore*, A. Di Stefano, G. Lucente, G. Luisi, B. Michelotto, G. Orlando, F. Pinnen (Chieti, Italy)

PB-053 **Approaches towards the design of new poly(ADP-ribose)polymerase (PARP) inhibitors**
E. Camaioni, G. Costantino, M. Marinozzi, A. Macchiarulo, R. Pellicciari (Perugia, Italy)

PB-054 **Design, synthesis and pharmacological evaluation of novel clozapine-based antipsychotics**
B. Capuano, I.T. Crosby, E.J. Lloyd (Parkville, Australia)

PB-055 **Chemical and pharmacological properties of antinociceptive naphthalene derivatives**
S. Collina, O. Azzolina, D. Vercesi, M. Nani, A. Barbieri, E. Lanza, C. Tadini, V. Ghislandi (Pavia, Italy)

PC-056 **Structure-activity studies of stereoisomers of antinociceptive naphthalene derivatives**
S. Collina, O. Azzolina, D. Vercesi, D. Rossi, A. Barbieri, E. Lanza, V. Ghislandi (Pavia, Italy)

PB-057 **Search for novel antidepressants through synergy between α_2 adrenoreceptor antagonism and monoamine uptake inhibition**
A. Cordi, I. Berque-Bestel, T. Persigand, J.-M. Lacoste, A. Newman Tancredi, A. Gobert, M. Brocco, J.-M. Rivet, M.J. Millan (Suresnes, France)

PB-058 **Development of a receptor interaction model for GABA-B ligands**
G. Costantino, A. Entrena Guadix, A. Macchiarulo, R. Pellicciari (Perugia, Italy)

PB-059 **2-Amino-9-alkylpurines – A new class of high affinity ligands for the benzodiazepine receptor**
K.S. Currie, P. Albaugh (Branford, USA)

PB-060 **Synthesis of some 1-(2-naphtyl)-2-(imidazole-1-yl)ethanone oxime ether derivatives and their anticonvulsant and antimicrobial activities**
A. Karakurt, *S. Dalkara*, M. Özalp, S. Özbey, E. Kendi, J.P. Stables (Ankara, Turkey)

PB-061 ***In vitro* stability, affinity and intrinsic activity studies of potential prodrugs for selective A_1 agonists**
A. Dalpiaz, C. Biondi, B. Pavan, F. Bortolotti, E. Durini, S. Manfredini (Ferrara, Italy)

PB-062 **Synthesis and potent anticonvulsivant activities of 4-oxo-10H-imidazo[1,2-a]indeno [1,2-e]pyrazin-2-carboxylic acid AMPA antagonists**
D. Damour, A. Böhme, A. Boireau, M-W. Debono, A. Genevois-Borella, P. Jimonet, J. Pratt, J.C.R. Randle, Y. Ribeill, J-M. Stutzmann, M. Vuilhorgne, S. Mignani (Vitry-sur-Seine, France)

PB-063 **Tryciclic theophylline derivatives**
A. Drabczynska, C. E. Müller, E. Pekala, S. Rockitt, H. Duddeck, J. Karolak-Wojciechowska, K. Kiec-Kononowicz (Krakow, Poland)

PB-064 **Adenosine analogs prodrugs: design, synthesis and chemico-physical characterization of N6-cyclopentyladenosine (CPA) derivatives**
S. Manfredini, P.G. Baraldi, *E. Durini*, F. Bortolotti, A. Scatturin, A. Dalpiaz (Ferrara, Italy)

PB-065 **New conformationally restrained tricyclic and tetracyclic melatonin analogs: design, synthesis and biological evaluation**
A. Eleutheriades, M. Vlachou, M. Panoussopoulou, A. Tsotinis, M.-T. Teh, D. Sugden (Athens, Greece)

PB-066 **2-(2-Oxo-1-azacycloalkyl)acetanilides as potential cognitive enhancers**
O. Farsa, K. Polachova, L. Benes (Brno, Czech Republic)

PB-067 **Design and synthesis of conformationally constrained analogs of L-glutamate and L-aspartate: potential inhibitors/substrates of excitatory amino acid transporters**
C. Fattorusso, M. De Angelis, S. Armaroli, G. Campiani, V. Nacci (Salerno, Italy)

PB-068 **Synthesis and pharmacological characterization of analogues of the GABA uptake inhibitor THPO**
B. Frølund, E. Falch, J. Perregaard, A. Schousboe, K. Frydenvang, P. Krogsgaard-Larsen (Copenhagen, Denmark)

PB-069 **Diarylmethylenepiperidine derivatives as selective glycine uptake inhibitors**
J. Clark, T.R. Clarkson, S.G. Gibson, I.G. Gilbert, *R. Gilfillan*, C. Howie, D.R. Jaap, D.R. Rae (Newhouse, Scotland)

PB-070 **Development of 2,3-benzodiazepines and related AMPA receptor antagonists**
R. Gitto, A. Chimirri, M. Zappalà, S. Quartarone, F. Bevacqua, A. De Sarro, G. De Sarro (Messina, Italy)

PB-071 **Synthesis and dopamine receptor binding of fused azaindole derivatives**
S. Löber, H. Hübner, *P. Gmeiner* (Erlangen, Germany)

PB-072 **Synthesis and SAR studies on acetylcholinesterase inhibitors**
A. Rampa, *S. Gobbi*, A. Bisi, L. Piazzi, F. Belluti, M. Bartolini, V. Andrisano, M. Recanatini, P. Valenti (Bologna, Italy)

PB-073 **7,8-Methylenedioxy-1,2,3,5-tetrahydro-4*H*-2,3-benzodiazepin-4-ones as novel noncompetitive AMPA receptor antagonists**
S. Grasso, S. Polimeni, M. Zappalà, A. De Sarro, G. De Sarro (Messina, Italy)

PB-074 **Selective M_4-agonists for treatment of pain**
G. Grewal, M.K. Alessi, C. Bayne, X. Cai, S. Cheah, J. Ellis, J. Eshraghi, R. Fisher, J. Grassi, T.A. Grinnell, W. Hao, B.E. Landgraf, G.M. Latham, B. Levine, H.A. Lounsbury, X. Liu, K.H. Nocka, R.T. Scannell, A. Toy-Palmer, D.W. Wypij, Z. Zhao, H-X. Zhai, F. Zuo (Cambridge, USA)

PB-075 **Design, synthesis, and conformational studies of new templates as ligands at melanocortin 3 and 4 receptors**
P. Grieco, E. Novellino, G. Greco, D. Weimberg, T. MacNeil, V.J. Hruby (Napoli, Italy)

PB-076 **Pharmacological behavior of two pyrazolo[5,1-c][1,2,4]benzotriazine 5-oxides-3-substituted, as new central BZR ligands**
A. Costanzo, *G. Guerrini*, G. Ciciani, F. Bruni, S. Selleri, C. Costagli, P. Malmberg-Aiello, C. Martini, B. Costa (Firenze, Italy)

PB-077 **Mixed 5-$HT_{1A/1B/1D}$ receptor antagonists as novel antidepressants**
M. Evans, S. Flynn, L.M. Gaster, L. Gordon, M.S. Hadley, M. Harries, *T.D. Heightman*, R. King, H.R. Marshall, J.P. Pilleux, J. Powles, G. Price, H. Rami, G. Riley, C. Roberts, C. Scott, R. Stead, J. Watson, S.L. White, P.A. Wyman (Harlow, UK)

PB-078 **Potent partial agonists for rat 5-HT_{2A} receptors: application of a new structure-activity concept**
R. Heim, H.H. Pertz, S. Elz (Berlin, Germany)

PB-079 **Development of a new structure-activity concept for partial 5-HT_{2A} -receptor agonists**
R. Heim, H.H. Pertz, S. Elz (Berlin, Germany)

PB-080 **Chiral analogues of ketanserin and altanserin: synthesis and potent 5-HT_{2A} -receptor antagonism on the rat tail artery**
T. Klaß, S. Elz (Berlin, Germany)

PB-081 **Chiral derivatives of pelanserin: synthesis and inversed stereoselectivity at the vascular rat 5-HT_{2A} -receptor**
T. Klaß, S. Elz (Berlin, Germany)

PB-082 **Tryciclic CRF receptor ligands**
R.F. Horvath, A.J. Hutchison (Branford, USA)

PB-083 **3-[3-(Piperazin-1-yl)propyl]indoles: agonists for the h5-HT_{1d} receptor with high selectivity over the h5-HT_{1b} receptor**
R.A. Jelley, S.C. Hobbs, A.M. MacLeod, A.J. Reeve, F. Sternfeld, L.J. Street, M.S. Beer, A. Heald, J.A. Stanton (Harlow, UK)

PB-084 **Search for novel nootropic drugs among azacrown-ethers with pharmacophore substituents**
T.L. Karaseva, N.G. Lukyanenko, S.S. Basok (Odessa, Ukraine)

PB-085 **Dependence of sulfonamides neurotropic activity from the character a carcass fragment of amine and amino group distante from the carbon carcass**
L.I. Kasyan, H.T. Zlenko, A.O. Kasyan, I.N. Tarabara (Dnepropetrovsk, Ukraine)

PB-086 **Diphenyl- and arylidene-substituted imidazo[2,1-b]-thiazoles and ring-enlarged homologs as ligands for the benzodiazepine binding site of $GABA_A$ receptors**
K. Kiec-Kononowicz, C.E. Müller, J. Karolak-Wojciechowska, B. Michalak, E. Pekala (Krakow, Poland)

PB-087 **Novel 2-phenylpurine derivatives as mitochondrial benzodiazepine receptor ligands**
K. Kondoh, T. Murata, K. Masumoto, K. Ohno, H. Kohayakawa, A. Kita, K. Furukawa (Osaka, Japan)

PB-088 **Novel, highly potent antioxidants**
M. Koufaki, T. Calogeropoulou, A. Detsi, A. Roditis, A. Kourounakis, K. Tsiakitzis, P. Kourounakis (Athens, Greece)

PB-089 **Design, synthesis and biological evaluation of a new series of allosteric enhancers of A_1-adenosine receptor**
I. Lampronti, P.G. Baraldi, N. Abdel Zaid, J.C. Shryock (Ferrara, Italy)

PB-090 **Effect of substituted 6-imidazo[2,1-b]thiazolylmethyl-2,3-dimetossi-5-methyl-benzoquinones on Complex I activity**
A. Leoni, A. Andreani, M. Rambaldi, R. Morigi, A. Locatelli, R. Fato, G. Lenaz (Bologna, Italy)

PB-091 **Synthesis and evaluation of the conformational aspect on the serotonin 5-HT_{1A} receptor affinity of a series of "long-chain" arylpiperazines**
M. Leopoldo, N.A. Colabufo, E. Lacivita, F. Berardi, R. Perrone, V. Tortorella (Bari, Italy)

PB-092 **A rational design of an intra-molecular hydrogen-bond to increase the CNS penetration of an NK_1 receptor antagonist**
V. Ashwood, J. Cook, M. Field, D.C. Horwell, C. Julien-Larose, *R.A. Lewthwaite*, M.C. Pritchard, J. Raphy, L. Singh (Cambridge, UK)

PB-093 **Affinity of new chiral aryloxyalkylpiperidines towards σ receptor subtypes**
F. Berardi, N.A. Colabufo, G. Fracchiolla, *F. Loiodice*, R. Perrone, V. Tortorella (Bari, Italy)

PB-094 **Pharmacophore model for anticonvulsant of α-substituted N-benzylamides of γ-hydroxybutyric acid**
B. Malawska, K. Kulig, J.P. Stables (Krakow, Poland)

PB-095 **Synthesis and activity of 3-pyridylamine ligands at central nicotinic receptors**
M. Marastoni, G. Balboni, P.A. Borea, R. Tomatis (Ferrara, Italy)

PB-096 **Molecular models of dopaminergic receptors**
A. Martinelli, G. Ortore, E. Di Gaddo (Pisa, Italy)

PB-097 **GSK-3 inhibitors: a new therapeutical strategy for neurodegeneration**
A. Martinez, C. Perez, A. Castro, F.J. Moreno, F. Wandosell (Madrid, Spain)

PB-098 **Design, synthesis and biological evaluation of new melatoninergic compounds**
C. Jellimann, M. Lefas-Le Gall, *M. Mathé-Allainmat*, J. Andrieux, S. Sicsic, J.P. Nicolas, J. Boutin, P. Delagrange, C. Bennejean, P. Renard, M. Langlois (Châtenay-Malabry, France)

PB-099 **Chain and fused carbonyl derivatives of 2-iminoimidazolidine with serotonergic activity**
D. Matosiuk, S. Fidecka, L. Antkiewicz-Michaluk (Lublin, Poland)

PB-100 **Synthesis, biochemical pharmacology, and evaluation of the excitotoxic efficacy of (S)-CPW399, a novel and selective AMPA agonist**
E. Morelli, A. Ramunno, R. Griffiths, C. Sinclair, H. Reavy, A. Cagnotto, T. Mennini, V. Nacci, G. Campiani (Siena, Italy)

PB-101 **Twin amides as potential prodrugs of L-DOPA**
B. Mosciatti, G.M. Cingolani, A. Di Stefano, G. Luisi, M. Ricciutelli, F. Claudi (Camerino, Italy)

PB-102 **Synthesis and cholinesterase activity of phenylcarbamates related to rivastigmine, a new therapeutical agent for Alzheimer's disease**
C. Mustazza, A. Borioni, M.R. Del Giudice, F. Gatta, A. Meneguez, T. Volpe (Roma, Italy)

PB-103 **Discovery of novel neuroprotectans, Na^+ and Ca^{2+} channel dual blockers with antioxidant activity**
H. Annoura, *K. Nakanishi*, T. Koba, N. Takemoto, S. Imajo, A. Miyajima, Y. Tamura-Horikawa, S. Tamura (Osaka, Japan)

PB-104 **Synthesis, SAR and biological activities of potent and selective group II metabotropic glutamate receptor agonists, novel 2-amino-fluorobicyclo[3.1.0]hexane-2,6-dicarboxylic acid derivatives**
A. Nakazato, T. Kumagai, K. Sakagami, R. Yoshikawa, Y. Suzuki, S. Chaki, S. Okuyama (Saitama, Japan)

PB-105 **Quantitative structure-retention relationships (QSRR) in a group of newly synthesized buspirone analogues**
A. Nasal, R. Kaliszan, Z. Chilmonczyk (Gdansk, Poland)

PB-106 **Novel 2,3,4,5-tetrahydro-1*H*-3-benzazepines and 2,3-dihydro-1*H*-isoindoles with high affinity and selectivity for the dopamine D_3 receptor**
D.J. Nash, K. Avenell, I. Boyfield, C. Branch, M.S. Hadley, C.N. Johnson, G. Macdonald, G.J. Riley, A.B. Smith, G. Stemp, K.M. Thewlis, A. Vong, M. Wood (Harlow, UK)

PB-107 **Oximethereal piperidinic derivatives: synthesis and affinity for serotonin and dopamine transporters**
A. Lapucci, E. Micali, *S. Nencetti*, S. Rapposelli, G.C. Demontis, M. Mazzoni (Pisa, Italy)

PB-108 **Synthesis of a novel series of tryciclic indan derivatives as melatonin agonists**
S. Ohkawa, O. Uchikawa, K. Fukatsu, R. Tokunoh, M. Kawada, K. Matsumoto, Y. Imai, K. Kato, H. Nishikawa, M. Miyamoto (Osaka, Japan)

PB-109 **New 4-substituted piperidine derivatives as antidepressants**
A. Toledo, M.C. Pumar, R. Mosquera, A. Innerárity, L. Labeaga, *A. Orjales* (Bilbao, Spain)

PB-110 **Synthesis and dopaminergic properties of the two enantiomers of 3-(3,4-dimethylphenyl)-1-propylpiperidine, a potent and selective dopamine D4 receptor ligand**
B. Macchia, L. Cervetto, G.C. Demontis, B. Longoni, M. Macchia, *E. Orlandini*, C. Papi (Pisa, Italy)

PB-111 **Structure-activity relationship study of asiatic acid derivatives against beta amyloid (Aβ)-induced neurotoxicity**
S.S. Jew, C.H. Yoo, D.Y. Lim, H. Kim, I. Mook-Jung, M.W. Jung, H. Choi, Y.H. Jung, H. Kim, *H.G. Park* (Seoul, Korea)

PB-112 **Synthesis of morpholinomethyl benzamides analogues of the antidepressant moclobemide**
H. Pessoa-Mahana, P.H.A. Lara, O.C. Astudillo (Santiago, Chile)

PB-113 **New NMDA receptor agonists and antagonists differ only by lipophylicity**
L.B. Piotrovsky, P.V. Lishko, O.A. Kryshtal, A.Yu. Bespalov (St. Petersburg, Russia)

PB-114 **An enantioselective synthesis and biobehavioral evaluation of 7-fluoro-3-(*p*-fluorophenyl)-2-propyltropanes**
K.R.C. Prakash, M. Trzcinska, K.M. Johnson, A.P. Kozikowsky (Washington, USA)

PB-115 **HPLC analysis of the novel antidepressant reboxetine in human plasma**
M.A. Raggi, G. Casamenti, R. Mandrioli, N. Ghedini, V. Volterra (Bologna, Italy)

PB-116 **Monitoring of plasma levels of clozapine and its metabolites by means of an HPLC method with coulometric detection**
M.A. Raggi, G. Casamenti, R. Mandrioli, C. Sabbioni, V. Volterra (Bologna, Italy)

PB-117 **Effect of combined administration of tryptophan, taurine and branched-chain amino acids on the pool of neuroactive compounds in rat brain structures after ethanol withdrawal**
Y. Razvodovsky, Y.M. Doroshenko (Grodno, Belarus)

PB-118 **New tropinone O-(arylpyrazolyl)propynyloximes and their muscarinic activities**
M.I. Rodríguez-Franco, *I. Dorronsoro*, G. Antequera, A. Martínez, C. Pérez, A. Badía, N.M. Vivas (Madrid, Spain)

PB-119 **1,4-Diazabicyclo[4.3.0]nonan-9-ones and 1,4-diaminopiperazines as new classes of highly potent nootropic drugs**
D. Manetti, C. Ghelardini, A. Bartolini, C. Bellucci, S. Dei, N. Galeotti, F. Gualtieri, *M.N. Romanelli*, S. Scapecchi, E. Teodori (Firenze, Italy)

PB-120 **Bis-tetrahydroacridine derivatives as AChE inhibitors**
L. Savini, A. Gaeta, L. Chiasserini, G. Campiani, C. Pellerano (Siena, Italy)

PB-121 **Pirazolo[3,4-b]piridines as A_1 adenosine ligands potentially attractive as neuroprotective agents**
S. Schenone, O. Bruno, A. Ranise, L. Mosti, F. Bondavalli (Genova, Italy)

PB-122 **Synthesis and neurotropic activity of silyl and tetrahydroisoquinolyl derivatives of thiazole**
I. Segal, A. Zabłocka, S. Germane, A. Geronikaki, K. Hatziopoulos, E. Lukevics (Riga, Latvia)

PB-123 **Different functionalities in dopamine D_3-receptor ligands related to BP 897**
H. Stark, S. Perachon, A. Mann, F. Garrido, C.G. Wermuth, J.-C. Schwartz, P. Sokoloff (Berlin, Germany)

PB-124 **Highly active and selective histamine H_3-receptor antagonists of the imoproxifan series**
H. Stark, A. Sasse, B. Sadek, X. Ligneau, S. Elz, H. Pertz, P. Luger, C.R. Ganellin, J.-M Arrang, J.-C Schwartz, W. Schunack (Berlin, Germany)

PB-125 **Benzophenone derivatives and related compounds as histamine H_3-receptor antagonists**
A. Sasse, X. Ligneau, S. Elz, C.R. Ganellin, J.-M Arrang, J.-C Schwartz, W. Schunack, *H. Stark* (Berlin, Germany)

PB-126 **Heterocyclic substituted 4-(3-(phenoxy)propyl)-1*H*-imidazoles as potent histamine H_3-receptor antagonists**
H. Stark, B. Sadek, X. Ligneau, J.-M. Arrang, C.R. Ganellin, J.-C Schwartz, W. Schunack (Berlin, Germany)

PB-127 **Resolution of ATPA and Thio-ATPA, two potent and selective GluR5 agonists**
T.B. Stensbøl, B. Nielsen, H.S. Jensen, K. Frydenvang, L. Borre, J. Egebjerg, T. Johansen, P. Krogsgaard-Larsen (Copenhagen, Denmark)

PB-128 **Y-931, a novel antipsychotic with potential anti-NRH (NMDA receptor-hypofunction) activity: synthesis and structure-activity relationships of 6*H*-[1]benzothieno-[2,3-*b*][1,5]benzodiazepines**
H. Tanaka, K. Kimura, H. Horiuchi, T. Kohara, M. Fujimura, K. Hashimoto, H. Yasumatsu, T. Morimoto, K. Yamagami, M. Arita (Saitama, Japan)

PB-129 **Synthesis of completely open-chain analogs of MK-801 as potent NMDA-receptor linked ion channel blockers**
S. Tkachenko, S. Bachurin, L. Petrova, A. Ustinov, A. Proshin, N. Zefirov (Chernogolovka, Russia)

PB-130 **Variation neurosecretory phenomenon of normal white rats and rats treated with mixture lidocaine+adrenaline in course of sexual cycle**
J. Tomin, V. Ivanovski, B. Lovic, D. Lovic, B. Stamenkovic, S. Glogovac, B. Stojkovic, R. Pavlovic (Nis, Yugoslavia)

PB-131 **New acetylcholinesterase inhibitors: *N*-benzylpiperidine ω-amidated dicarboxylic amino acid derivatives**
S. Conde, *M.-P. Torres-Candela*, C. Pérez, A. Castro, A. Martínez (Madrid, Spain)

PB-132 **Synthesis of a novel series of benzocycloalkene derivatives as melatonin agonists**
O. Uchikawa, K. Fukatsu, M. Kawada, T. Yamano, M. Yamashita, K. Kato, M. Miyamoto, S. Ohkawa (Osaka, Japan)

PB-133 **Synthesis of the pyrazolotriazinone derivative AWD 34-022 and its pharmacological profile**
T. Arnold, H.-J. Lankau, A. Rostock, *K. Unverferth* (Radebeul, Germany)

PB-134 **New N, N' –disubstituted piperazines as serotonine and dopamine ligands**
E. Estrada, J.C. González, L. Santana, *E. Uriarte*, Y. Fall, C. Terán, I. Loza (Santiago de Compostela, Spain)

PB-135 **Enone prodrugs of hydroxylated aminotetralins: PD148903, derivatives and analogs**
B.J. Venhius, H.V. Wikström, D. Wustrow, L. Meltzer, L.D. Wise, S. Johnson, D. Dijkstra (Groningen, The Netherlands)

PB-136 **Synthesis of polycilic pyrrolopyridines as melatonin receptor ligands**
H. Van De Poel, P. Renard, C. Bennejean, P. Delagrange, J.A. Boutin, J.P. Nicolas, G. Guillaumet, *M.-C. Viaud* (Tours, France)

PB-137 **New prolyl oligopeptidase inhibitors**
E.A.A. Wallén, J.A.M. Christiaans, M. Forsberg, P.T. Männistö, J. Gynther (Kuopio, Finland)

PB-138 **Synthesis and stability of dopamine prodrugs**
S. Zanarone, A. Sala, R. Ippolito, M.G. Rimoli, E. Abignente, P. de Caprariis, G. Boatto (Napoli, Italy)

PB-139 **Organosilicon polyaddition polymers for medicine**
S. Nanushyan, *E. Alexeeva*, A. Artem'ev (Moscow, Russia)

PB-140 **Theoretical studies and synthesis of N-(1,2,5,7-dithiadiazonan-6-yliden)cianamide. A new immunostimulant compound**
E. Angeles, I. Menconi, G. Ordoñez, A. Romero, R. Martínez, R. López-Castañares (Mexico)

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PB-141 **Resolution of 2-arylpropionic acid esthers using lipase enzyme**
B. Berk, H. Akgün (Ankara, Turkey)

PB-142 **Stereochemical characterisation of potential cocaine antagonists by enantioselective HPLC and circular dicroism detection**
C. Bertucci, V. Andrisano, R. Gotti, M. Roberti, D. Simoni (Bologna, Italy)

PB-143 **Fullerenes in medicinal chemistry**
S. Bosi, T. Da Ros, M. Bergamin, V. Tomberli, B. Baiti, C. Cusan, F. Pellarini, G. Spalluto, M. Prato (Trieste, Italy)

PB-144 **Design and synthesis of tricyclic adenosine analogues**
D. Camp, R.J. Quinn, U. Wermuth (Melbourne, Australia)

PB-145 **Characterisation of novel CYP2C9 and CYP2D6 substrates for fluorescence P450 assays**
R. Elliott, R. Bambal, J.C. Bloomer, R.J. Chenery, S.E. Clarke, C. Leach (Harlow, UK)

PB-146 **Chemistry, pharmacology and clinical studies of novel antidepressant peptides**
J.J. Hlavka, H. Abajian, G. Nicolau, J.P. Feighner (Suffern, USA)

PB-147 **Resolution of racemic ibuprofen by using two-component resolving agent**
X. Hu, G. Li, J. Wen, J. Li, Q. Hu, X. Gong, J. Shu (Wuhan, China)

PB-148 **Pharmaexpert: knowledge-based computer system for discovery of new drugs**
A. Lagounine, V. Poroikov, D. Filimonov (Moscow, Russia)

PB-149 **SAR by crystallography: a new approach combining screening and rational drug design. Application to the discovery of nanomolar Src SH2 binders**
D. Lesuisse, P. Deprez, D. Bénard, P. Broto, G. Delettre, V. Jean-Baptiste, J.P. Marquette, E. Sarubbi, B. Schoot, E. Mandine, G. Lange (Romainville, France)

PB-150 **Peptide analogues of a Epstein-Barr virus LMP2-derived epitope**
M. Marastoni, M. Bazzaro, S. Salvadori, R. Guerrini, R. Gavioli, F. Micheletti, R. Tomatis (Ferrara, Italy)

PB-151 **New solid supported reagents (SSRs) for amines acylation**
E. Petricci, M. Botta, F. Corelli, M. Renzulli (Siena, Italy)

PB-152 **Automated solid phase synthesis of 3-hydroxy methyl and 3-carbamyl methyl isoxazoles**
M. Quai, W. Barbaglia, A. Ezhaya, E. Cereda (Milano, Italy)

PB-153 **Correlations between fundamental characteristics of the "organism-drug" system**
S.A. Silantiev, V.G. Zinkovsky, N.Y. Golovenko, O.V. Zhuk, S.I. Zchukin (Odessa, Ukraine)

PB-154 **Automated, high throughput analysis of dissolution samples by HPLC**
M.E. Swartz, P.M. Young, K. Johnson, P.A. Fowler (Milford, USA)

PB-155 **Synthesis of nucleoside 3'-*O*-(*S*-p-nitro-phenyl methanephosphonodithioate)S and *O*-(*Se*-p-nitrophenyl methanephosphonoselenothioate)S**
L.A. Wozniak, A. Chworos, W.J. Stec (Lodz, Poland)

PB-156 **Methanephosphonoanilidothioate approach to stereocontrolled chemical ligations**
L.A. Wozniak, J. Pyzowski, W.J. Stec (Lodz, Poland)

Session C: Friday, September 22

PC-003 **Novel efficient methods for synthesis of adducts of oligonucleotides with highly hydrophobic molecules**
S. I. Antsypovich, S.Yu. Andreev, T.S. Oretskaya, Z.A. Shabarova (Moscow, Russia)

PC-004 **Study of the distribution in mouse of furocoumarins and an angelicin isoster**
R. Bevilacqua, F. Baccichetti, A. Guiotto (Padova, Italy)

PC-005 **Synthesis, antitubercular activity and pharmacophore fitting of new derivatives of toluidine**
M. Biava, R. Fioravanti, G.C. Porretta, G. Sleiter, D. Deidda, G. Lampis, R. Pompei, A.Tafi, F. Manetti (Roma, Italy)

PC-006 **Spectroscopic investigation of the metal – ligand coordination in some diclofenac complexes**
Gh. Bora, I. Bratu, O. Cozar, M. Bora, *V. Bora* (Cluj-Napoca, Romania)

PC-007 **Unexpected *in vivo* gastroprokinetic activity of benzoic ester derivatives of 4-hydroxymethylpiperidines**
J.-P.R. Bosmans, A.L. Meulemans, H.H. Bohets, C.J. Love, M.A. De Cléyn, M.G. Verdonck, E.C. Ghoos, M. Jurzak, J.A. Schuurkes (Beerse, Belgium)

PC-008 **Conformational analysis of a new series of indole derivatives ligand of the serotonine receptors**
C. Saturnino, A. Capasso, *M. Buonerba*, G. Barone, G. De Martino (Salerno, Italy)

PC-009 **New activators of BK_{Ca} potassium channels**
G. Biagi, *V. Calderone*, I. Giorgi, O. Livi, C. Manera, V. Scartoni, B. Baragatti, E. Martinotti (Pisa, Italy)

PC-010 **Synthesis of some Mannich N-bases of triazoloquinolines as pharmacologically active compounds**
M.G. Ferlin, G. Chiarelotto (Padova, Italy)

PC-011 **Synthesis and *in vitro* antimycobacterial activity of sulconazole analogs**
R. Fioravanti, M. Biava, G.C. Porretta, D. Deidda, C. Maullu, R. Pompei (Roma, Italy)

PC-012 **Liquid chromatographic (HPLC) determination with fluorescence detection of B_6 vitamers and riboflavin in multivitamin preparations and milk**
M.G. Gioia, *R. Gatti* (Bologna, Italy)

PC-013 **Reversible carnitine palmitoyltransferase inhibitors with antidiabetic activity. 2. Aminocarnitine derivatives**
A. Arduini, G. Calvisi, R. Catini, P. Chiodi, F. De Angelis, E. De Fusco, N. Dell'Uomo, G. Gallo, *F. Giannessi*, D. Meloni, P. Pessotto, E. Tassoni, M.O. Tinti (Roma, Italy)

PC-014 **Synthesis and pharmacophore generation of new pyridazinone derivatives with affinity towards α_1-α_2 adrenoceptors**
G. Strappaghetti, S. Corsano, R. Barbaro, G. Giannaccini, L. Betti, M. Botta, F. Manetti, *L. Maccari* (Siena, Italy)

PC-015 **An oxorhenium-RGD derivative complex for radiopharmaceutical application**
V. Kostopoulos, *M. Pelecanou*, E. Mikros, C.I. Stassinopoulou, A.D. Varvarigou, S.C. Archimandritis (Athens, Greece)

PC-016 **Synthesis and characterization of thiocolchicoside derivatives**
A. Sacchi, S. Laneri, M. Gallitelli, M. Iadanza, E. Abignente, P. Colombo, P. Santi (Napoli, Italy)

PC-017 **Substrates and inhibitors of human tissue kallikrein containing unconventional amino acids**
V. Santagada, G. Caliendo, E. Perissutti, F. Fiorino, B. Severino, L. Juliano (Napoli, Italy)

PC-018 **1,8-Naphthyridine derivatives: potent and selective A_1 adenosine antagonists**
P.L. Ferrarini, C. Mori, C. Manera, G. Saccomanni, *S. Simi*, L. Betti, G. Giannaccini, A. Lucacchini (Pisa, Italy)

PC-019 **Synthesis and evaluation of adenosine transporter inhibitors**
H. Takai, S. Fujiwara, Y. Okamura, H. Nonaka, H. Kase, K. Yao, A. Karasawa (Shizuoka-ken, Japan)

PC-020 **Reversible carnitine palmitoyltransferase inhibitors with antidiabetic activity. 1. Broad chemical diversity**
L. Almonte, A. Arduini, G. Calvisi, R. Catini, P. Chiodi, F. De Angelis, E. De Fusco, N. Dell'Uomo, F. Giannessi, F. Giorgi, I. Lustrati, M. Mabilia, M. Marzi, P. Minetti, S. Muck, P. Pessotto, *E. Tassoni*, M.O. Tinti (Roma, Italy)

PC-021 **Bifunctional complexes of rhenium (I) and technetium (I) containing chemotactic sequences: chemistry and biological studies**
A. Lazzaro, A. Dalpiaz, A. Scatturin, A. Marchi, *G. Vertuani* (Ferrara, Italy)

PC-022 **Synthesis of new class of platinum(II) complexes with captoprile as a potential antitumor agents**
M. Aleksic, *D. Agbaba*, D. Milojkovic-Opsenica, Z. Tesic, S. Radulovic (Belgrade, Yugoslavia)

PC-023 **Alkylating agents from sugars. Glycosyl glycerols as chlorambucil carrier systems**
F. Alcudia, J.M. Vega-Pérez, J.I. Candela, I. Romero, E. Blanco, F. Iglesias-Guerra (Sevilla, Spain)

PC-024 **A general enantiodivergent synthesis of C_2-symmetric 1,2-ethane-bis-sulfoxides**
N. Khiar, *F. Alcudia*, C.S. Araújo, I. Fernández (Sevilla, Spain)

PC-025 **Pyrazolo[3,4,5-*kl*]acridine-5-carboxamides: a new class of potential antitumor agents with excellent antiproliferative activity**
I. Antonini, A. Magnano, P. Polucci, S. Martelli (Camerino, Italy)

PC-026 **Cytotoxic activity of silyl and germyl substituted 4,4-dioxo-3a,6a-dihydrothieno-[2,3-*d*]isoxazolines-2**
P. Arsenyan, O. Pudova, I. Shestakova, E. Lukevics (Riga, Latvia)

PC-027 ***Ab initio* study of the structure of N-diphenylmethyl-2-propenamide**
G. Barone, C. Saturnino, G. De Martino, G. La Manna, D. Duca (Salerno, Italy)

PC-028 **Trimeric naphthoquinones as antiviral agents**
D.G. Bourke, J.A.V. Coates, M.P. Collis, *I.T. Crosby*, P.J. de Bruyn, P.L.C. Keep, M.L. Rose, A.D. Robertson (Parkville, Australia)

PC-029 **Phenyl sulfur mustard derivatives of distamycin A**
I. Beria, M. Caldarelli, L. Capolongo, P. Cozzi, C. Geroni, S. Mazzini, E. Ragg (Milano, Italy)

PC-030 **Interaction of cytotoxic distamycin derivatives with plasmidic DNA**
I. Beria, M. Caldarelli, P. Cozzi, C. Geroni, A. Cirla, S. Mazzini, E. Ragg (Milano, Italy)

PC-031 **Arylazoenamines endowed with antiproliferative activity**
V. Boido, C. Canu Boido, F. Sparatore, S. Doratiotto, D. Delpiano, P. La Colla (Genova, Italy)

PC-032 **Antiproliferative activities of variously substituted 2-phenyl- and 2-benzyl-benzimidazoles**
V. Boido, L. Mina, F. Sparatore, G. Paglietti, S. Doratiotto, M.G. Setzu, D. Delpiano, P. La Colla (Genova, Italy)

PC-033 **A new class of synthetic quinonic compounds acting as antiproliferative agents**
A. Bolognese, T. Di Meo, M. Manfra, G. Correale, O. Mazzoni, E. Novellino, G. Brunetti, L. Sanna, D. Delpiano, P. La Colla (Napoli, Italy)

PC-034 **2,3-Dihydro-1H-imidazo[1,2-b]pyrazole derivatives with potential antiproliferative activity**
S. Schenone, O. Bruno, A. Ranise, *F. Bondavalli* (Genova, Italy)

PC-035 **Oxophosphonates – A new class of potent matrix metalloproteinase inhibitors**
R. Reich, C.J. Salomon, Y. Katz, W. Chen, A. Goldblum, *E. Breuer* (Jerusalem, Israel)

PC-036 **Phosphorylated analogs of 4-hydroxytamoxifen**
T. Calogeropoulou, M. Koufaki, A. Detsi, I. Fichtner, G. Eisenbrand, D. Syriani, M.N. Alexis, H.R. Hendriks, A. Makriyannis (Athens, Greece)

PC-037 **QSAR of bispyridinium compounds: antiproliferative agents via inhibition of choline kinase**
J. Campos, M.C. Núñez, A. Entrena, V. Rodríguez, M.A. Gallo, A. Espinosa (Granada, Spain)

PC-038 **QSAR/QSPR correlations of novel anticancer drugs: π–electron-delocalized lipophilic biscations**
J. Campos, M.C. Núñez, R.M. Sánchez, A. Conejo, M.A. Gallo, A. Espinosa (Granada, Spain)

PC-039 **Cytotoxic diterpenylnaphthohydroquinones. Structural modifications at the terpenic moiety**
M.A. Castro, J.M. Miguel del Corral, M. Gordaliza, P. Chamorro, M.D. García-Grávalos, A. San Feliciano (Salamanca, Spain)

PC-040 **Synthesis and preliminary in vitro anticancer activity of new uracil derivatives**
M.T. Cocco, *C. Congiu*, V. Onnis, R. Piras (Cagliari, Italy)

PC-041 **Synthesis and cytotoxic activity of benzodioxinic derivatives**
S. Clavier, *G. Coudert*, D.H. Caignard, P. Renard, A. Pierré, G. Atassi (Orléans, France)

PC-042 **Benzoisoquinolinquinone and cyclobuten naphtoquinone derivatives: synthesis and antiproliferative activity**
M.V. Diurno, P. Campiglia, G. Correale, G. Gatta, I. Gomez-Monterrey, O. Mazzoni, L. Sanna, M.G. Setzu, I. Serra, D. Delpiano, S. Doratiotto, P. La Colla (Napoli, Italy)

PC-043 **New tetracyclic frameworks with potential antitumor interest**
E. Estrada, J.C. Gonzales, J. Lobo-Antunes, E. Quezada, L. Santana, E. Uriarte (Santiago de Compostela, Spain)

PC-044 **A new prototype of symmetrical bis(5-fluorouracil-*O,N*-acetals) with two amide bonds**
M.A. Gallo, J.F. Domínguez, J.A. Marchal, J. Prados, J. Campos, A. Aránega, A. Espinosa (Granada, Spain)

PC-045 **Synthesis and antitumor activity of 3-alkoxy analogues of flavone-8-acetic acid**
S. Gobbi, A. Rampa, A. Bisi, F. Belluti, P. Valenti, A. Caputo, M. Carrara (Bologna, Italy)

PC-046 **Synthesis and biological evaluation of cytotoxic monoterpenylnaphthoquinones**
M. Gordaliza, M.A. Castro, J.M. Miguel del Corral, M.L. Martín-Martín, M.D. García-Grávalos, A. San Feliciano (Salamanca, Spain)

PC-047 **Synthesis and evaluation of novel steroidal oxime inhibitors of P450 17 (17α-hydroxylase / C17-20-lyase) and 5 α-reductase type 1 and 2**
S. Haidar, M. Hector, P.B. Ehmer, W. Reichert, J. Jose, R.W. Hartmann (Saarbrücken, Germany)

PC-048 **Synthesis and cytostatic effects of bis-(alpha-benzyl)-azatyrosylamides on human cancer cell lines**
M.-K. Hu, C.-F. Lu (Taipei, Taiwan)

PC-049 **Synthesis and *in vitro* cytotoxicity of hexacyclic camptothecin analogues**
S.S. Jew, H.J. Kim, M.G. Kim, E.Y. Roh, J.K. Kim, J.H. Lee, H. Lee, H.G. Park (Seoul, Korea)

PC-050 **Discovery and optimization of chromanes as new potent P21-Ras competitive farnesyltransferase inhibitors**
P. Jimonet, B. Baudoin, A. Lebrun, J.F. Sabuco, Y. El-Ahmad, A. Genevois, F. Clerc, O. Angouillant, J.D. Guitton, A. Laoui, S. Pickett, S. Maignan, J.P. Guilloteau, J.F. Riou, Y. Lelièvre, L. Debussche, A. Commerçon, N. Dereu (Vitry-sur-Seine, France)

PC-051 ***N*-substituted 3-aryl-2-quinolones: synthesis and putative use in cancer chemotherapy**
B. Joseph, F. Darro, R. Kiss, B. Lesur, A. Frydman, G. Guillaumet (Orléans, France)

PC-052 **Hologram QSAR analysis of propafenone-type modulators of multi-drug resistance**
D. Kaiser, P. Chiba, G. Ecker (Wien, Austria)

PC-053 **Levan of *Zymomonas Mobilis* - the nonspecific immunomodulator of cancer**
I. Vina, *A. Karsakevich*, A. Zhilevica, R. Treimane, M. Bekers (Riga, Latvia)

PC-054 **Synthesis and properties of glycoconjugates, containing two anticancer agents - L-asparaginase and polyfructose levan**
A. Karsakevich, I. Vina (Riga, Latvia)

PC-055 **Pyrazolo[3,4-b]pyridines: potent inhibitors of cyclin-dependent kinases**
R.N. Misra, R. Batorsky, I. Bursuker, C. Chang, K.A. Kellar, *S.D. Kimball*, J.G. Mulheron, D.B. Rawlins, J.S. Sack, W. Shan, J. Tokarski, K. Webster, H. Xiao (Princeton, USA)

PC-056 **Synthesis, conformational analysis and cytotoxic activity of some new pyrano[3,2-*b*]thioxanthen-6-ones and pyrano[2,3-*c*]tioxanthen-7-ones**
I.K. Kostakis, N. Pouli, P. Marakos, E. Mikros, A.L. Skaltsounis, S. Leonce, Gh. Atassi, P. Renard (Athens, Greece)

PC-057 **The design and synthesis of a pyrazolo[3,4-*c*]pyridine C-nucleoside as potential antitumor agent**
V. Kourafalos, P. Marakos, N. Pouli, L.B. Townsend (Athens, Greece)

PC-058 **7H-Pyrrolo[3,2-c]imidazo[1,2-e]pyrimidin-2(3H)-one a new tricyclic DNA-interactive ring system**
A. Lauria, P. Diana, P. Barraja, G. Dattolo, G. Cirrincione, A.M. Almerico (Palermo, Italy)

PC-059 **Synthesis and potential coanthracyclinic activity of imidazo[2,1-b]thiazole guanylhydrazones**
A. Locatelli, R. Morigi, A. Leoni, M. Rambaldi, M. Recanatini, A. Andreani, V. Garaliene (Bologna, Italy)

PC-060 **Synthesis of R116010, a retinoic acid (RA) metabolism inhibitor with antitumoral effects**
D. Mabire, M. Venet, G. Sanz, H. Poignet, W. Wouters, J. Van Wauwe (Val de Reuil, France)

PC-061 **Ceramide analogues as a new strategy for anticancer drug development**
M. Macchia, S. Barontini, S. Bertini, R. Danesi, M. Del Tacca, V. Di Bussolo, S. Fogli, E. Giovannetti, E. Grossi, F. Minutolo (Pisa, Italy)

PC-062 **Aroylpyrrole-acylhydroxamates: a new class of histone deacetylase inhibitors**
A. Mai, G. Sbardella, S. Massa, R. Ragno, G. Brosch (Roma, Italy)

PC-063 **Design, synthesis and activity of a new class of highly selective human mitochondrial thymidine kinase inhibitors**
S. Manfredini, P.G. Baraldi, E. Durini, L. Porcu, A. Angusti, N. Solaroli, E. De Clercq, A. Karlsson, J. Balzarini (Ferrara, Italy)

PC-064 **Design, synthesis and activity of phosphono-acetic bioisosters of ribofuranosylnucleoside diphosphates as potential RNR inhibitors**
S. Manfredini, P.G. Baraldi, E. Durini, *L. Porcu*, S. Vertuani, N. Solaroli, A. Verri, S. Spadari, F. Focher, E. De Clercq, J. Balzarini (Ferrara, Italy)

PC-065 **The synthesis and pharmacological evaluation of a new potent daunomycinone derivative**
N. Aligiannis, N. Pouli, *P. Marakos*, A.L. Skaltsounis, S. Mitaku, H. Pratsinis (Athens, Greece)

PC-066 **Synthesis of new indolo[3,2-c][1,8]naphthyridine derivatives as antiproliferative agents**
A. Da Settimo, G. Primofiore, F. Simorini, A.M. Marini, F. Da Settimo, L. Dalla Via, O. Gia, *S. Marciani Magno* (Padova, Italy)

PC-067 **Naphthyl combretastatin A-4 analogues**
A.B.S. Maya, B. Del Rey, E. Caballero, M.D. García-Grávalos, *M. Medarde*, A. San Feliciano (Salamanca, Spain)

PC-068 **Novel 7-imino- and oximinomethylenecamptothecins with potent in vitro and in vivo antitumor activity**
S. Dallavalle, B. Biasotti, A. Ferrari, *L. Merlini*, G. Gallo, M. Marzi, S. Penco, C. Pisano, N. Carenini, P. Perego, M. De Cesare, G. Pratesi, F. Zunino (Milano, Italy)

PC-069 **Synthesis and antitumor activity of 4-hydroperoxy derivatives of ifosfamide and its bromo analogues**
K. Misiura, S. Szymanowicz, H. Kusnierczyk, A. Opolski, J. Wietrzyk, A. Siwinska (Lódz, Poland)

PC-070 **Indolylmethylene- and imidazo[2,1-b]thiazolylmethylene-2-indolinones. A new class of CDK1/cyclin B inhibitors**
R. Morigi, A. Locatelli, A. Leoni, M. Rambaldi, A. Andreani, M. Recanatini, A. Cavalli, M. Garnier (Bologna, Italy)

PC-071 **New steroid sulfatase inhibitors**
P. Nussbaumer, A. Billich (Vienna, Austria)

PC-072 **Synthesis of enantiomerically pure 1-[α-benzofuran-2-yl)arylmethyl]1,2,4-triazoles, antifungal and antiaromatase agents**
A. Paladino, F. Messina, M. Botta, F. Corelli (Siena, Italy)

PC-073 **New antitumoral agents derived from pyrido[2,3-*d*]pyrimidines**
J.A. Palop, C. Sanmartín, M.V. Domínguez, M. Font, M.E. Ardaiz, M. Echeverría, B. Mendivil, A. Martín, J. García-Foncillas, I. Okroujnov, E. Dudich (Pamplona, Spain)

PC-074 **Novel combretastatin analogues with two trimethoxyphenyl rings**
R. Pelaez Lamamie de Clairac, M. Medarde (Salamanca, Spain)

PC-075 **Conformationally restricted analogues of combretastatones**
J.E. Hernàndez, *R. Pelaez Lamamie de Clairac*, M. Medarde (Salamanca, Spain)

PC-076 **Nonsteroidal inhibitors of 5 α-reductase. Synthesis of N-substituted piperidine-4-(benzylidene-4-carboxylic acids) and evaluation of type 1 and 2 isozyme inhibition**
F. Picard, R.W. Hartmann (Saarbrücken, Germany)

PC-077 **Dioxygenated xanthones: effect on human cancer cell lines and human T-lymphocyte proliferation**
M.M.M. Pinto, M.S.J. Nascimento, *M. Pinto*, E. Sousa, M. Pedro, F. Cerqueira (Porto, Portugal)

PC-078 **Quinoxalines analogues-omologues of classical antifolates**
S. Piras, M. Loriga, G. Paglietti (Sassari, Italy)

PC-079 **Preparation and cytotoxic activity of some new rhodomycine derivatives bearing modifications in the sugar part**
N. Aligiannis, *N. Pouli*, P. Marakos, A.L. Skaltsounis, S. Mitaku, J.C. Florent, E.M. Perchellet, B.J. Sperfslage, C.J. McIlvain, J.P. Perchellet (Athens, Greece)

PC-080 **Synthesis and antitumor activity of benzimidazolinium salts**
O. Pudova, P. Arsenyan, I. Shestakova, E. Lukevics (Riga, Latvia)

PC-081 **Platinum(II) and palladium(II) complexes of usnic acid condensation products and their cytostatic activity**
S. Radulovic, Z. Juranic, M. Mandic, D. Sladic, K. Andjelkovic, Z. Tesic (Belgrade, Yugoslavia)

PC-082 **A new class of potent apoptotic agents (PBOX) based on an oxazepine scaffold: identification of potential antitumor agents**
A. Ramunno, C. Fattorusso, D. Zisterer, C. Williams, M. Mc Gee, V. Nacci, G. Campiani (Salerno, Italy)

PC-083 **Benzoyl nitrogen mustard derivatives of pyrazole analogues of distamycin A: synthesis and antileukemic activity**
R. Romagnoli, P.G. Baraldi, B. Cacciari, G. Spalluto, I. Beria, P. Cozzi, C. Geroni, N. Mongelli (Ferrara, Italy)

PC-084 **SAR analysis of the cellular influx and cytotoxicity of aminopterin analogs with a nonpolyglutamatable side chain**
A. Rosowsky, J.E. Wright, C.M. Vaidya, R.A. Forsch (Boston, USA)

PC-085 **Synthesis and cytotoxicity of organosilicon derivatives of pyridine and quinoline sulfides and amidoximes**
K. Rubina, E. Abele, R. Abele, P. Arsenyan, I. Sleiksa, I. Shestakova, E. Lukevics (Riga, Latvia)

PC-086 **Novel functionalized pyrido[2,3-*g*]quinoxalin-2-ones as antibacterial, antifungal and anticancer agents**
A. Carta, *P. Sanna*, L. Gherardini, A. Deriu, L. Sechi, S. Zanetti (Sassari, Italy)

PC-087 **A new class of heterocyclic-containing arotinoids endowed with potent differentiating and apoptotic activity**
D. Simoni, M. Roberti, R. Rondanin, M. Rossi, R. Baruchello, S. Grimaudo, M. Tolomeo, D. Arindam, D. Benbrook (Ferrara, Italy)

PC-088 **Programmed cell death associated with the stilbene motif of arotinoids: discovery of novel aminoarotinoids possessing potent apoptotic activity**
D. Simoni, F.P. Invidiata, M. Roberti, R. Rondanin, R. Baruchello, M. Rossi, C. Malagutti, A. Mazzali, S. Grimaudo, M. Tolomeo, N. D'Alessandro (Ferrara, Italy)

PC-089 **Comparative molecular field and comparative molecular similarity analysis of propafenone-type modulators of multi-drug resistance**
M. Smiesko, P. Chiba, G. Ecker (Bratislava, Slovakia)

PC-090 **Kielcorin derivatives: effect on human cancer cell lines and human T-lymphocyte proliferation**
M.M.M. Pinto, M.S.J. Nascimento, *E. Sousa*, M. Pedro, F. Cerqueira (Porto, Portugal)

PC-091 **Structure activity relationships in a series of potent MDR inhibitors**
E. Teodori, S. Dei, A. Garnier-Suillerot, P. Gratteri, F. Gualtieri, D. Manetti, M.N. Romanelli, S. Scapecchi (Firenze, Italy)

PC-092 **New analytical investigations concerning the role of superoxide dismutase in kidney cancer**
L. Campanella, L. Persi, R. Grossi, *M. Tomassetti* (Roma, Italy)

PC-093 **Design and synthesis of potential $P450_{AROM}$ and 17β-HSD inhibitors for the treatment of breast cancer**
T. Vinh, C. Simons (Cardiff, UK)

PC-094 **Pyrrolo[1,2-a]quinoxalines analogues of antifolic methotrexate and trimetrexate**
P. Corona, *G. Vitale*, M. Loriga, S. Alleca, G. Paglietti (Sassari, Italy)

PC-095 **Synthesis and MDR-modulating activity of enantiopure 1-benzopyrano[3,4-*b*]-[1,4]oxazines**
P. Wetwitayaklung, P. Chiba, G. Ecker (Wien, Austria)

PC-096 **Cryptolepine-related analogs as potent antifungal agents**
S.Y. Ablordeppey, P.C. Fan, A. Nimrod, A.M. Clark (Tallahassee, USA)

PC-097 **Synthesis and antimicrobial activity of new 3-methyl-5-(5-methyl-1*H*-1-R'-3-pyrazolyl)-1*H*-1-R-4-nitrosopyrazoles. Part III**
E. Aiello, *S. Aiello*, F.P. Invidiata, D. Simoni, F. Mingoia, M.G. Setzu, I. Serra, G. Brunelli, L. Sanna, P. La Colla (Palermo, Italy)

PC-098 **Synthesis of new 6-bromopenicillanic acid derivatives as potential β-lactamase inhibitors**
A. Bedini, G. Tarzia, B. Di Giacomo, G. Gatti, C. Balsamini, B. Citterio, L. Giorgi (Urbino, Italy)

PC-099 **Disubstituted N-imidazolamines and their "carba-analogues" as antifungal agents**
S. Castellano, G. Stefancich, G. Setzu, P. La Colla (Trieste, Italy)

PC-100 **6-Desfluoroquinolones: antimycobacterial activity and NAD synthetase inhibition**
V. Cecchetti, O. Tabarrini, M. Rizzi, G. Riccardi, G. Cruciani, A. Fravolini (Perugia, Italy)

PC-101 **Insights into molecular recognition interactions at the teicoplanin binding site**
S. Cellamare, C. Maccallini, P. Iuliani, C. Altomare, M. Ferappi, A. Carotti (Chieti, Italy)

PC-102 **Synthesis, antibacterial, and cytotoxic evaluation of certain 7-substituted norfloxacin derivatives**
C.-C. Tzeng, K.-C. Fanf, Y.-L. Chen (Kaohsiung, Taiwan)

PC-103 **Mini–library of diaza-boronic acids as AmpC beta-lactamase inhibitors**
V. Buzzoni, B. Shoichet, J. Blasquez, *M.P. Costi* (Modena, Italy)

PC-104 **Thymidylate synthase inhibitors as antimicrobial agents: high rate hits discovery through combinatorial approach**
M.P. Costi, S. Ferrari, M. Ingrami, P. Pecorari, D. Tondi, M. Rinaldi (Modena, Italy)

PC-105 **Isoxazolo[3,4-d]pyridazinones and analogues as Leishmania mexicana PDE inhibitors**
V. Dal.Piaz, A. Rascon, C. Vergelli, M.E. Dubra, M.P. Giovannoni, C. Castellana (Firenze, Italy)

PC-106 **RNase P inhibitors as potential antibacterial agents**
D. Dean, S. Davies, A. Gaiba, M. Gress, P. Ham, L. Hegg, F. King, G. Jones, A. Naylor, J. Park, N. Pearson, S. Rittenhouse, J. Seal, A. Takle, D. Wilson (Essex, UK)

PC-107 **Synthesis of new C-6 alkyliden penicillin derivatives as potential beta-lactamase inhibitors**
B. Di Giacomo, G. Tarzia, A. Bedini, G. Gatti, C. Balsamini, W. Baffone, F. Bartoccini (Urbino, Italy)

PC-108 **Activated nitriles in heterocyclic synthesis part II: pyrimido[3,4a]benzimidazoles, pyrazolopyrimidobenzimidazoles, 2-oxazinyl and 2-pyrazolylbenzimidazoles as antimicrobial agents**
M. El-Kerdawy, H. Hammad, G. Nawar, L. Shabaka (Mansoura, Egypt)

PC-109 **Synthesis and biological evaluation of N-substituted-pyridin-4-thiones**
M.D. Aytemir, R.C. Hider, *D.D. Erol*, M. Özalp (Ankara, Turkey)

PC-110 **Design, synthesis and evaluation of N-substituted-3-hydroxypyridin-4-ones with antimicrobial activities**
M.D. Aytemir, R.C. Hider, *D.D. Erol*, M. Özalp (Ankara, Turkey)

PC-111 **Synthetic analogues of the natural product SB-219383: potent inhibitors of bacterial tyrosyl tRNA synthetase**
R.L. Jarvest, J.M. Berge, P. Brown, R.C. Haltiwanger, D.W. Hamprecht, D.J. McNair, C.S.V. Houge-Frydrych, L.M. Mensah, P.J. O'Hanlon, A.J. Pope, S. Rittenhouse (Harlow, UK)

PC-112 **Stable analogues of physiological allylic prenyl diphosphates as inhibitors of mycobacterial prenyl diphosphate synthases**
M. Macchia, S. Barontini, D.C. Crick, P.J. Brennan, C. Papi, M.C. Schulbach (Pisa, Italy)

PC-113 **Stereoselective synthesis of 5-substituted-3-pyrrol-1-yl-2-oxazolidinones as useful tool to design novel potential antibacterial and CNS agents**
A. Mai, M. Artico, G. Sbardella, S. Massa, F. Demontis, R. Loddo, D. Delpiano, P. La Colla (Roma, Italy)

PC-114 **Synthesis and antimycobacterial activity of substituted 2,4-dihydro-1,2,4-triazole-3-thione and 3*H*-thiazol-2-ylidene-hydrazide derivatives**
M.G. Mamolo, D. Zampieri, V. Falagiani, E. Tonzar, L. Vio, E. Banfi (Trieste, Italy)

PC-115 **Synthesis and antifungal activity of imidazole linked 4,5-dihydro-1*H*-pyrazole derivatives**
M.G. Mamolo, V. Falagiani, D. Zampieri, E. Tonzar, L. Vio, E. Banfi (Trieste, Italy)

PC-116 **Quinoline piperidines as novel anti-bacterial agents**
R.E. Markwell, D. Davies, M. Gwynn, C. Henry, A. Hodgson, F. King, A. Naylor, A. Takle, N. Pearson, S. Rittenhouse (Harlow, UK)

PC-117 **Antifungal activity of new arylbenzothiazoles group**
J. Matysiak, Z. Kleinrok, *D. Matosiuk*, A. Niewiadomy, A. Koziol (Lublin, Poland)

PC-118 **Synthesis and *in vitro* anti-*Mycobacterium* activity of new quinoxaline 1,4-di-*N*-oxides and 2-quinoxalinecarbonitriles**
Y. Sainz, F.J. Martínez-Crespo, M.E. Montoya, M.A. Ortega, I. Aldana, A. López de Cerain, *A. Monge* (Pamplona, Spain)

PC-120 **Synthesis and antibacterial activity of pyridazino[4,3-b]indole-4-carboxylic acids**
F. Palluotto, F. Campagna, A. Carotti, G. Casini, A. Rosato, C. Vitali (Bari, Italy)

PC-121 **SAR for the lipophilic derivatives of glycopeptide antibiotic eremomycin**
A.Y. Pavlov, M.N. Preobrazhenskaya (Moscow, Russia)

PC-122 **Antimycobacterial and antiproliferative evaluation of aryl- and heteroaryl-derivatives of the (benzotriazol-1(2)-yl) acrylonitrile**
P. Sanna, A. Carta, M.E. Rahabar Nikookar, M.E. Setzu, M.G. Brunetti, P. La Colla (Sassari, Italy)

PC-123 **Novel trisubstituted quinoxalines-1,4-dioxide as antibacterial, antifungal and antiprotozoal agents**
M.E. Rahabar Nikookar, *P. Sanna*, A. Carta, G. Paglietti, L. Sechi, P.L. Fiori, S. Zanetti (Sassari, Italy)

PC-124 **Interaction of antimicrobic drug ethonium with DNA, homopolynucleotides and their monomers**
V.A. Sorokin, V.A. Valeev, G.O. Gladchenko (Kharkov, Ukraine)

PC-125 **Synergistic effect of HE/NE laser and gentamicin on alginate production in Pseudomonas Aeruginosa**
E. Souri, P. Owlia, Q. Behzadian-nejad (Tehran, Iran)

PC-126 **Synthesis and *in vitro* activity of novel antituberculous compounds. Study of the pharmacokinetic profile**
M. Terreni, M. Pregnolato, D. Ubiali, G. Pagani, J.L. Pedraz Muñoz, A. Rodríguez Gascón (Pavia, Italy)

PC-127 **Pyrazolo[3,4-*d*][1,3]thiazine and pyrazolo[1,5-*c*][1,3,5]thiadiazine derivatives as potential antifungal agents**
C.B. Vicentini, M. Manfrini (Ferrara, Italy)

PC-128 **Synthesis and antiviral activity of quinolone and oxazine derivatives**
A. Bolognese, P. Cerruti, G. Nese, M. Manfra, G. Correale, O. Mazzoni, E. Novellino, D. Delpiano, G. Setzu, G. Brunetti, P. La Colla (Napoli, Italy)

PC-129 **Synthesis and biological evaluation of a new heterodinucleotide with anti-HIV activity**
P. Franchetti, L. Cappellacci, M. Grifantini, L. Rossi, S. Serafini, M. Magnani, C.-F. Perno (Camerino, Italy)

PC-130 **The new data of arbidol activity**
R. Glushkov, T. Guskova, A. Shuster, I. Leneva, L. Krylova (Moscow, Russia)

PC-131 **The discovery of substituted pyrrolidine human CCR5 receptor antagonists possessing anti-HIV activity**
J.J. Hale, S.G. Mills, M. MacCoss, P.E. Finke, R.J. Budhu, E.B. Holson, M.S. Springer, L. Malkowitz, W.A. Schleif, A. Carella, G. Carver, E. Emini (Rahway, USA)

PC-132 **Chromosomal abnormalities analysis in B-CLL leukemia cells by fluorescent in situ hybridization**
D. Koczkodaj, D. Rozynkowa, A. Filip, M. Gawlowicz, B. Marzec, U. Gasowska, J. Wojcierowski (Lublin, Poland)

PC-133 **A chemoenzymatic approach to the synthesis of a neuraminidase inhibitor based on the lincosaminide scaffold**
A.M. Maione (Roma, Italy)

PC-134 **Synthesis, in vitro and in vivo anti-HSV1 activity of N,N'-bispyrimidyl dispirotripiperazine**
V. Makarov, A. Stelzner, M. Schmidtke (Moscow, Russia)

PC-135 **Selective inhibitors of Sendai virus: pharmacophore model generation**
F. Manetti, F. Corelli, R. Saladino, M. Botta (Siena, Italy)

PC-136 **Pseudopeptide N-hydroxyamides as HIV-1 protease inhibitors**
M. Marastoni, M. Bazzaro, S. Salvadori, R. Guerrini, R. Tomatis (Ferrara, Italy)

PC-137 **Activity of DABOs against clinically relevant HIV-1 resistant mutants**
T. Marceddu, F. Demontis, L. Vargiu, A. Mai, G. Sbardella, M. Artico, P. La Colla (Cagliari, Italy)

PC-138 **Potent non-nucleoside inhibitors of human cytomegalovirus: benzothiadiazine dioxide (BTD) dibenzyl derivatives**
A. Martinez, C. Gil, C. Perez, A. Castro, M.I. Abasolo, A. Bruno, C. Prieto, J. Otero, G. Andrei, R. Snoeck, J. Balzarini, E. De Clercq (Madrid, Spain)

PC-139 **Benzimidazole derivatives: role of cyclofunctionalization on selectivity against HIV-1 or HIV-2**
A. Chimirri, E. De Clercq, *A.M. Monforte*, P. Monforte, L. Musumeci, C. Pannecouque, A. Rao, M. Witvrouw, M. Zappalà (Catanzaro, Italy)

PC-140 **Synthesis of 3'-modified nucleosides as potential anti-HIV**
C. Montagnani, F. Corelli, M. Botta, C. Mugnaini (Siena, Italy)

PC-141 **Cross-resistance pattern of DABO-resistant mutants**
C. Musiu, A.G. Loi, F. Demontis, A. Mai, G. Sbardella, M. Artico, P. La Colla (Cagliari, Italy)

PC-142 **Fluoren β-O-glucosides: biosynthesis and DNA-intercalating activity evaluation**
R. Ottanà, D. Macchione, R. Maccari, F. Monforte, A. Trincone, S. Alcaro, M.G. Vigorita (Messina, Italy)

PC-143 **Tilorone analogues with IFN-inducing and anti-HSV-2 activity**
D. Macchione, M.G. Vigorita, *R. Ottanà*, R. Maccari, S. Alcaro, A. Speranza, A. Arena (Messina Italy)

PC-144 **Synthesis of spiro-pyranocoumarins with potential anti-HIV activity**
V. Panteleon, P. Marakos, N. Pouli, A.L. Skaltsounis, E. Mikros (Athens, Greece)

PC-145 **Physico-chemical properties and antiviral activity of streptokinase, pyruvate kinase and streptokinase-pyruvate kinase complex**
N.I. Pavlova, O.N. Murashko, O.V. Savinova, E.I. Boreko, V.N. Nikandrov (Minsk, Belarus)

PC-146 **Antiviral activity of adducts of fullerene C_{60} with polyvinylpyrrolidone**
L.B. Piotrovsky, O.I. Kiselev, K.N. Kozeletskaya, M.A. Dumpis, L.N. Posnjakova (St. Petersburg, Russia)

PC-147 **Imidazopyridines as potential NNRTIs: synthesis and biological evaluation**
G. Pürstinger, J. Balzarini, E. De Clercq, C. Pannecouque, M. Witvrouw (Innsbruck, Austria)

PC-148 **A predictive model for HIV non-nucleoside reverse transcriptase inhibitors (NNRTIs)**
R. Ragno, M. Artico, G.R. Marshall (Roma, Italy)

PC-149 **Binding mode and structure based drug design of new DABO derivatives**
R. Ragno, M. Artico, A. Mai, G. Sbardella, S. Massa, D. Delpiano, R. Loddo, G. Brunetti, M.G. Setzu, P. La Colla (Roma, Italy)

Session C: Friday, September 22

PC-150 **N,N-disubstituted dihydro-alkylamino-benzyl-oxopyrimidines, a new class of potent and selective anti-HIV-1 agents belonging to DABOs**
G. Sbardella, A. Mai, M. Artico, S. Massa, M.G. Setzu, R. Loddo, I. Serra, G. Brunetti, P. La Colla (Roma, Italy)

PC-151 **Is HSV1 TK selective for fixed forms of sugar ring pucker?**
L. Scapozza, P. Schelling, P. Pospisil, J. Vogt, V. Marquez, A. Prota, G.E. Schulz, G. Folkers (Zurich, Switzerland)

PC-152 **Synthesis and biological activity of indole-2-diketo acids as HIV-1 integrase inhibitors**
M. Sechi, G. Paglietti, Dallocchio, L. Sanna, G. Brunetti, P. La Colla (Sassari, Italy)

PC-153 **Synthesis, anti-HIV-1 RT activity and binding mode of 1-[2-(diarylmethoxy)ethyl]-2-methyl-5-nitroimidazoles (DAMNIs)**
R. Silvestri, M. Artico, G. De Martino, R. Ragno, S. Massa, I. Serra, F. Demontis, G. Brunatte, S. Doratiotto, P. La Colla (Roma, Italy)

PC-154 **New amino- and hydrazinoacridines: design, synthesis and biological activity**
Y.I. Suveyzdis, H.A. Lyakhoya, S.A. Lyakhov, L.A. Litvinova, S.A. Andronati (Odessa, Ukraine)

PC-155 **3D-QSAR study of quinolones as anti-HIV agents**
V. Cecchetti, *O. Tabarrini*, E. Filipponi, G. Cruciani, A. Fravolini (Perugia, Italy)

PC-156 **New 1,1,3-trioxo-thieno[3,4-*e*][1,2,4]thiadiazines (TTDs). Synthesis and anti-HIV-1 activity**
M.T. Molina, X. Liu, *S. Vega*, V. Gomez Parra, M. Witvrouw, C. Pannecouque, J. Balzarini, E. De Clercq (Madrid, Spain)

PC-157 **Molecular interactions in enzymes: a DFT approach. Sugar binding to HSV TK**
M. Sulpizi, G. Folkers, L. Scapozza, F. Alber, P. Carloni (Trieste, Italy)

PC-158 **Design and synthesis of potent Src SH2 selective inhibitors with *in vivo* osteoclast anti-resorptive activity**
R. Sundaramoorthi, W. Shakespeare, C. Metcalf, Y. Wang, C. Vu, T. Merry, C. Haroldson, U. Mani, S. Pradeepan, R. Bohacek, D. Dalgarno, S. Narula, M. Hatada, M. R. van Schravendijk, S. Adams, S. Violette, J. Smith, W. Guan, C. Bartlett, J. Iuliucci, F. Cerasoli, M. Weigele, T. Sawyer (Cambridge, USA)

GENERAL INFORMATION

Venue

The Symposium will be held at

Palazzo della Cultura e dei Congressi
Piazza Costituzione 4
40128 Bologna, Italy
Tel.: +39 051 6375111
Fax: +39 051 6375170
E-mail: bocongressi@alinet.it

Registration and Information Desk

The registration desk will be located in the entrance hall of the Conference Centre. It will be open frc 15.00 on Monday, 18 September, and will remain open during the week whilst the scientific sessio are in progress.

Information Board

General information and announcements will be displayed on an information board in the entrance h of the Conference Centre, next to the registration desk.

Personal Messages

Messages and incoming mail will be held at the registration desk. During the days of the Symposiu mail for participants should be addressed to the individual at the following address:

Palazzo della Cultura e dei Congressi
Piazza Costituzione 4
40128 Bologna, Italy
Tel.: +39 051 6375111
Fax: +39 051 6375170
E-mail: bocongressi@alinet.it

Symposium Language

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

Admission Badge

Each participant will be supplied with a clip-on name badge. For security reasons, participants a asked to wear their badges at all times whilst in the Conference Centre.
For the purpose of identification, the following colour scheme will be used:

Symposium Participants	White
Single Day Participants	Pink
Accompanying Persons	Yellow
Executive Committee	Blue
Secretariat	Red
Exhibitors	Green

GENERAL INFORMATION

Application

Attendance at any part of the Symposium, including the Accompanying Person's programme, is restricted to those who have applied in advance. The closing date for application is **August 31, 2000.**
All applications should be made on the Application Form (which can be downloaded from http://www.scfarm.unibo.it/bo2000) and returned with the appropriate remittance. All cheques/money orders should be made payable to **Planning Congressi Srl.** Completed applications should be sent to the Congress Secretariat:

Planning Congressi Srl
Via S. Stefano 97, 40125 Bologna (Italy)
Tel. +39 051 302980-81 – Fax +39 051 309477 – E-mail: info.planning@planning.it

If for any reason it is necessary to send the remittance separately from the Application Form, every care should be taken to ensure that the cheque/money order includes both the **title of the meeting** and **the individual** concerned. All applications received at Planning Congressi Srl will be acknowledged.

Fees

The registration fees (inclusive of 20% VAT) are:

Standard Registration: After May 31, 2000

➢ Industrialists	Euro	720
➢ Academics	Euro	720
➢ IUPAC members	Euro	720
➢ Students*	Euro	360
➢ Daily attendance	Euro	160
➢ Accompanying Persons	Euro	150

* Students registration is only accepted after receipt of a letter of endorsement of the supervisor together with the registration form.

The registration fee for Participants to the Symposium includes:
admission to scientific sessions, Abstract book, Proceedings book (to be mailed after the symposium), Welcome Cocktail Party (Monday, September 18, 2000), Concert (Tuesday, September 19, 2000), four lunches, seven coffee-breaks.
The Gala Dinner (Thursday, 21 September) has not been included in the registration fee and should be paid separately. The cost of the Gala Dinner is Euro 50.-.

The registration fee for daily attendance includes:
admission to scientific sessions for the selected day, Abstract book, one lunch, two coffee breaks.

The registration fee for Accompanying Persons includes:
Welcome Cocktail Party (Monday, September 18, 2000), Concert (Tuesday, September 19, 2000), guided visit of Bologna (Tuesday, September 19, 2000).
The Gala Dinner (Thursday, September 21, 2000) has not been included in the registration fee and should be paid separately. The cost of the Gala Dinner is Euro 50.-.
Similarly, lunches have not been included in the Accompanying Persons registration fee. For Accompanying Persons who wish to book for lunches the tickets will be available at the Registration Desk. The cost of the lunches will be Euro 23.- per day.

GENERAL INFORMATION

Payment

Payment can be made to the following account:

Planning Congressi Srl
no. 291/14 - ABI 05387.6 - CAB 02598.1
at Banca Popolare dell'Emilia Romagna - Ag. 6
Via Massarenti 228, 40138 Bologna (Italy)

Participants are reminded that bank charges are made and are deducted by the bank before passing the Congress Secretariat; it is therefore essential that such transfer of money should include a surcharge. Deductions suffered by the Congress Secretariat should be paid at the Registration Desk arrival. Please attach a copy of the payment advice to the Application Form.

Credit card payment of fees must be made in full and the following credit cards are acceptable: Vi Eurocard, Mastercard. The Congress Secretariat regrets that American Express and Diners cannot accepted. The particular card to be debited, together with the **Account Number, Expiry Date**, and **Registered Name** and **Address** of the Card Holder, must be specified on the Application Form.
It is quite in order for multiple applications to be made on one form provided all individ requirements are clearly indicated. Xerox copies of Application Forms are acceptable, as are fa applications.

All data supplied by participants will be processed and held on computer by the Congress Secreta only for the purpose of administering this conference.

Applications may be cancelled by **August 31, 2000** in which case a partial refund will be made. It v **not be possible** to offer any refunds if details of cancellation are received after that date.

Visas

Participants should check with their own local travel agents whether they will require a visa travelling to Italy. If so, they are advised to apply to the nearest Italian Embassy or Consulate at le two months before the intended date of travel.

IUPAC

IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provic application is made not less than three months in advance. If a visa is not granted one month before meeting, IUPAC Secretariat should be notified without delay by the applicant.

Letter of Invitation

On request, the Symposium chairman will be pleased to send personal invitations to prospect participants for XVIth International Symposium on Medicinal Chemistry. Such invitations are only the purpose of assisting participants to raise travel funds or obtain visas. No financial commitment the part of the organisers is implied. Requests should be sent to the Congress Secretariat Planni Congressi.

Technical Services

All meeting rooms will be equipped with video projectors for Power Point presentations and sli projectors for single or double projection. Overhead projectors and pointers will be available.

Slides must be 50x50 mm with an image window of 24x36 mm in plastic or metal mounts and protected by glass. All slides must bear a serial number and identification of the correct direction of insertion.

Slides (lectures and oral communications) must be submitted at least 60 minutes before presentation to the Slide Centres which will be located near to the meeting rooms.

Telephones

Participants are kindly requested to switch off mobile phones during the scientific sessions.

Poster Sessions

Posters will be on display in the foyers of the Conference Centre during the poster sessions as indicated in the programme. The authors are requested to mount their own poster on the board marked with their number as listed in the abstract book before 9.00 on the day of the session and remove it at the end of the session. The organizers cannot be held responsible for damage or loss of posters which are not removed on time.

Proceedings

The Proceedings of the Symposium containing the inaugural, plenary and main lectures will be published early in 2001. Each participant will receive a copy upon publication.

Abstracts

A Book of abstracts of all papers presented at the Symposium will be handed out to the participants at registration.

Meals and Refreshments

The cost of lunches on Tuesday, Wednesday, Thursday and Friday has been included in the Registration Fee for the meeting. All lunches will be served in a dedicated area where admission will be by presentation of lunch tickets only.

The cost of lunches has not been included in the fee for Accompanying persons. A limited number of tickets will be on sale at the Registration desk (Cost: 23 Euro).

No formal arrangements have been made for dinners. It is assumed that participants will make individual arrangements for eating.

Coffees and teas will be available in a dedicated area at the times specified in the scientific programme.

Special Diet/Disability

Special diet can be provided only if advance notice is given to Organisers. The Organisers are anxious to assist wherever possible with special needs in respect of any disability and requirements.

Exhibition

The Symposium foresees an associated exhibition of books and companies with goods and services relevant to the needs of Medicinal Chemists. Companies interested in taking part are invited to contact:

Planning Congressi Srl
Via S. Stefano 97, 40125 Bologna (Italy)
Tel. +39 051 302980-81 – Fax +39 051 309477 – E-mail: info.planning@planning.it

or

Prof. Ettore Novellino
Dipartimento di Chimica Farmaceutica e Tossicologica
Via Domenico Montesano 49 - 80131 Napoli (Italy)
Tel. +39 081 678643 - Fax +39 081 678644 - E-mail: novellin@unina.it

Accommodation

Those participants who wish to book hotel accommodation in Bologna can do so through **Bolog Congressi Convention and Travel.**

The Accommodation/Tourist Form (which can be downloaded fr http://www.scfarm.unibo.it/bo2000) and relevant deposit for accommodation (one night in the cho category) plus Euro 10.33 per room as agency fee, should be sent **by August 31, 2000** to:

Bologna Congressi Convention and Travel
Piazza Costituzione 5/e – 40128 Bologna (Italy)
Tel. +39 051 6375111/107 – Fax +39 051 6375149 – E-mail: bocongressi@alinet.it

If for any reason it is necessary to send the remittance separately from the Accommodation/Tou Form, every care should be taken to ensure that the cheque/money order includes both the **title of meeting** and **the individual** concerned.

Price per room: *(bed and breakfast, taxes included)*		**single room**	**double room**
Cat. A	(**** stars)	Euro 154.94-165.27	Euro 206.59-237.57
Cat. B	(****/*** stars)	Euro 90.38-139.44	Euro 129.11-170.43
Cat. C	(*** stars)	Euro 77.47-103.29	Euro 103.29-154.94

All requests will be satisfied on a "first come, first served" basis. Bologna Congressi Convention Travel reserves the right to assign the room according to the availability left.

All requests received at Bologna Congressi Convention and Travel will be acknowledged.

Payment can be made to the following account:

Bologna Congressi Convention and Travel
no. 313/9 - CAB 2407 – ABI 6385 Swift Code CRBOIT2B
at Cassa di Risparmio in Bologna – Fil. Fiera
Piazza Costituzione 8, 40128 Bologna (Italy)

Participants are reminded that bank charges are made and are deducted by the bank before passing Bologna Congressi Convention and Travel; it is therefore essential that such transfer of money sho include any surcharge. Deductions suffered by Bologna Congressi Convention and Travel should paid directly to the Hotel upon departure. Please attach a copy of the payment advice to Accommodation Form.

GENERAL INFORMATION

Credit card payment of fees must be made in full and the following credit cards are acceptable: Visa, Eurocard, Mastercard. Bologna Congressi Convention and Travel regrets that American Express and Diners cannot be accepted. The particular card to be debited, together with the **Account Number, Expiry Date**, and the **Registered Name** and **Address** of the Card Holder, must be specified on the Accommodation Form.

All data supplied by participants will be processed and held on computer by Bologna Congressi Convention and Travel only for the purpose of administering this conference.

Reservations may be cancelled by **August 31, 2000** in which case a partial refund will be made. It **will not be possible** to offer any refunds if details of cancellations are received after that date.

Correspondence

For Registration and Administrative Matters
Planning Congressi Srl
Via S. Stefano 97, 40125 Bologna (Italy)
Tel. +39 051 302980-81 – Fax +39 051 309477 – E-mail: info.planning@planning.it

For Accommodation and Tourist Programme
Bologna Congressi Convention and Travel
Piazza Costituzione 5/e – Bologna (Italy)
Tel. +39 051 6375111/107 – Fax +39 051 6375149 – E-mail: bocongressi@alinet.it

For Information about Exhibition
Prof. Ettore Novellino
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Via Domenico Montesano 49 - 80131 Napoli (Italy)
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or

Planning Congressi Srl
Via S. Stefano 97, 40125 Bologna (Italy)
Tel. +39 051 302980-81 – Fax +39 051 309477 – E-mail: info.planning@planning.it

For Advice on the Scientific Programme
Prof. Carlo Melchiorre, Symposium Chairman
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Useful Websites

Congress Website:	http://www.scfarm.unibo.it/bo2000
Bologna Conference Centre Website:	http://www.bolognacongressi.it
Bologna Website:	http://www.nettuno.it/bologna/TouringBologna

TOURIST INFORMATION

The City of Bologna

Bologna is at a natural cross-roads between northern, southern, eastern and western Italy, halfw between the Tyrrhenian coast to west and the Adriatic coast to east.
The city, which boasts one of the best preserved historical centre in the world, has about 40 kilomet of porticoed streets, where shoppers and tourists can shelter from the sun or from the rain. A number medieval palaces are clustered around Piazza Maggiore, the main central square, and around the chu of San Petronio, founded in 1390, which had been planned to be bigger than St Peter's, in Ron Slightly further away are the twelfth century leaning Asinelli and Garisenda towers, two of the f survivors of the 200 towers which once dominated the skyline of the medieval city.
Further evidence of the rich cultural history of Bologna can be seen in its many other church monuments, museums and in its University, the oldest one in the world, founded in 1088.
Bologna is warm and welcoming, its people are hospitable and fun loving, as any visitor will discov however short his stay in this town renowned also for its excellent cuisine.

How to get to Bologna

Bologna can be easily reached by all means of transport:

By air: The "Guglielmo Marconi" international airport has direct links with major centres in Euro (including Amsterdam, Barcelona, Brussels, Copenhagen, Frankfurt, Lyon, Lisbon, London, Madr Münich, Nice, Oporto, Paris, Prague and Vienna) and with the rest of the world via the intercontinen airports of Milan Malpensa and Rome Leonardo da Vinci.
Bologna airport is located about 9 km from the city centre and 7 km from the Conference Centre a has excellent coach and taxi connections.

By rail: The Eurostar train service links Bologna with more than 40 European cities, including Mil and Rome. Bologna railway station is located in the city centre, at a walking distance from the ma hotel area and about 3 km from the Conference Centre.

By road: Bologna is a major intersection for Italy's extensive motorway network. From the ring ro take exit 7 signposted Via Stalingrado and proceed to Piazza Costituzione (Palazzo della Cultura e c Congressi).

Public transportation

The Palazzo della Cultura e dei Congressi, which is located at the heart of one of the most importa trade fair complexes in Europe, is only a few minutes away from the city historical centre.
Public transports are available as follow:

- from the city centre: bus n. 18 and 10
- from the railway station: bus n. 38 and 10.

Parking

Several car parks are available all around the Conference Centre. Piazza Costituzione Car park, in tl immediate surrounding of the Palazzo della Cultura e dei Congressi, has a capacity of 650 cars.

Credit cards

Major credit cards (American Express, Diners Club, Mastercard, Visa) are accepted in most hotel restaurants and shops.

TOURIST INFORMATION

Foreign exchange

Most city banks exchange foreign currency and traveller's cheques. Opening hours: from 8.20 to 13.15 and from 14.30 to 15.30 from Monday to Friday. Some banks are also open all day either on Monday or Wednesday from 8.20 to 17.50. A bank office is available next to the Conference Centre.

Insurance

All participants are advised to make their own travel and health care insurance. The organisers will not be liable for any accident, theft and damage to property, nor for any delays or modification in the programme due to unforeseen circumstances.

Dress/Climate

The average temperature in September ranges from 23 °C during the day to 15 °C at night.
There is no formal dress for the evening social functions, with the exception of the Gala Dinner where jackets and ties for men will be considered appropriate.

SOCIAL PROGRAMME

The following social events are planned for all registered Participants and Accompanying Persons.

Admission to all events will be by ticket only, and tickets will be issued only if the appropri indication is given on the Application Form. All tickets should be collected by Participants registration on arrival.

Monday, September 18, 2000

Welcome Cocktail Party	18.30-20.30	Ticket: free

Tuesday, September 19, 2000

Guided Visit of Bologna (only for Accompanying Persons)	09.30-12.30	Ticket: free
Concert	21.00-22.30	Ticket: free

Wednesday, September 20, 2000

There are no scientific sessions on Wednesday afternoon. Possible excursions have been plann including tours with dinner (see Tourist Programme)

Thursday, September 21, 2000

Gala Dinner	20.00-23.30	Ticket: Euro 50.-

TOURIST PROGRAMME

The following excursions are planned for Accompanying Persons, and for Congress Participants (only on Wednesday, September 20, 2000 afternoon).

The participation to all excursions is restricted to those who have **applied in advance.** The closing date for application is **August 31, 2000.** Maximum and minimum numbers are fixed for all excursions, and participants are therefore requested to indicate an alternative choice on the application form to facilitate any reallocation if necessary. The Organisers reserve the right to cancel excursions if lack of demand (a minimum of **15 participants** is requested).

All applications should be made on the Accommodation/Tourist Form and returned with the appropriate remittance to **Bologna Congressi Convention and Travel.** All requests received at Bologna Congressi Convention and Travel will be acknowledged.

Participation to all excursions will be by ticket only, and tickets will be issued only if the appropriate indication is given on the Accommodation/Tourist Form. All tickets should be collected by Participants at registration on arrival.

Tuesday, September 19, 2000

Ferrara 14.30-18.30

Located only 40 km north of Bologna, Ferrara is a surprise for the visitor that sees it for the first time.

The historical centre is a place to be enjoyed by strolling around and by discovering its quiet beauty. The famous Estense family lived in Ferrara, and the castle, in the main square, is one of the many monuments to be visited.

Ticket: Euro 72.30/person

Wednesday, September 20, 2000

Guided visit of Bologna 14.30-18.30

The old town center is marvellously intact and its famous porticoes – a distinctive feature for which Bologna is world famous –meander for some 40 km along medieval streets, opening out onto charming piazzas and breathtaking monuments.

Further evidence of the rich cultural history of Bologna can be seen in its many other churches, museums and in its University, the oldest one in the world, founded in 1088.

Ticket: Euro 10.50/person

or

TOURIST PROGRAMME

Ferrara with dinner 14.30-23.00

Located only 40 km north of Bologna, Ferrara is a surprise for the visitor that sees it for the first time.

The historical centre is a place to be enjoyed by strolling around and by discovering its quiet beauty. The famous Estense family lived in Ferrara and the castle, in the main square, is one of the many monuments to be visited.

Ticket: Euro 92.97/person

or

Ravenna with dinner 14.30-23.00

Located on the Adriatic coast, Ravenna is a small city which accumulates magnificent architecture and constructions due to its ancient and glorious past.

Its monuments are known all over the world and its name is synonym for mosaic and Byzantine art.

Ticket: Euro 103.30/person

Thursday, 21 September, 2000

Venice with lunch 8.00-18.30

The name of this wonderful and unique city, built on 118 islands, has always enchanted and fascinated the world.

Its monuments that appear to the eyes of the visitor in an intangible interplay of light and colour, help to explain why the "Venetian Art" finds in light and colour its inner essence.

Ticket: Euro 118.80/person

or

Florence with lunch 8.30-18.30

City of balance and harmony, Florence is with its monuments one of the most famous art city in the world.

All forms of architecture, from churches to public buildings and down to the simpler houses, are informed by a strict rationalism which detests waste, exaggeration and rhetoric.

Ticket: Euro 108.50/person

PROGRAMME OVERVIEW

	Time-table	Europauditorium	Sala Topazio	Sala Italia
Monday September 18	15.00-17.00	Registration		
	17.00-17.30	Opening		
	17.30-18.30	Inaugural Lecture		
	18.30-20.30	Welcome Cocktail		
Tuesday September 19	08.00-09.00	Registration		
	09.00-09.45	PL1		
	10.00-10.25	ML5	ML9	ML1
	10.30-11.00	Coffee Break		
	11.00-12.25	ML6 – ML8	ML10 - ML12	ML2 – ML4
	12.30-12.45	OC2	OC3	OC1
	12.50-14.00	Lunch		
	14.00-14.55	ML21, ML22	ML13, ML14	ML17, ML18
	15.00-15.30	Coffee Break		
	15.30-16.25	ML23, ML24	ML15, ML16	ML19, ML20
	16.30-18.00	**Poster Session A**		
	21.00-22.30	Concert (Chiesa dei Servi, Strada Maggiore)		
Wednesday September 20	09.00-09.45	PL2		
	10.00-10.25	ML29	ML25	ML33
	10.30-11.00	Coffee Break		
	11.00-12.25	ML30 – ML32	ML26 – ML28	ML34 – ML36
	12.30-12.45	OC5	OC4	OC6
Thursday September 21	09.00-09.55	ML37, ML38	ML45, ML46	ML53, ML54
	10.00-10.30	Coffee Break		
	10.30-11.25	ML39, ML40	ML47, ML48	ML55, ML56
	11.30-12.25	OC7- OC9		OC10 – OC12
	12.30-14.00	Lunch		
	14.00-14.55	ML41, ML42	ML49, ML50	ML57, ML58
	15.00-15.30	Coffee Break		
	15.30-16.25	ML43, ML44	ML51, ML52	ML59, ML60
	16.30-18.00	**Poster Session B**		
	20.00-23.00	Gala Dinner (Villa Cicogna, San Lazzaro di Savena)		
Friday September 22	09.00-09.45	PL3		
	09.50-10.20	Coffee Break		
	10.25-11.20	OC16 - OC18	OC19 – OC21	OC13 – OC15
	11.25-13.00	**Poster Session C**		
	13.00-14.00	Lunch		
	14.00-14.55	ML68, ML69	ML61, ML62	ML64, 65
	15.00-15.25	Coffee Break		
	15.25-16.30	ML70, ML71	OC22,OC23, ML63	ML66, ML67
	16.35	Closing		

PL: plenary lecture; ML: main lecture; OC: oral communication