The 2nd Brazilian Symposium on Medicinal Chemistry

Current Trends in Drug Discovery and Development

2º Simpósio Brasileiro em Química Medicinal

Tendências Atuais na Descoberta e Desenvolvimento de Fármacos

Military Institute of Engineering - IME

Rio de Janeiro – Brazil, November 22-25, 2004

Instituto Militar de Engenharia - IME

Rio de Janeiro, 22 a 25 de Novembro de 2004

http://www.brazmedchem.ifsc.usp.br
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Universidade Federal de Minas Gerais (UFMG)
Advisor to the Chair

The 2nd Brazilian Symposium on Medicinal Chemistry

Scientific Program

November 22 (Monday)

4:30– 6:00 pm	**Registration at the Symposium Venue**
Opening Session	
6:30 – 7:00 pm	Jose Daniel Figueroa Villar, Brazil **Welcome from the Conference Chair**
Opening Conference	
	Anibal E. Vercesi, Brazil **Introduction of Speaker**
7:00 – 8:00 pm	George L. Kenyon, USA **Creatine Kinase: Structure and function of an Energetic Enzyme**
8:10 – 10:10 pm	**Social Event: Welcome Get-Together Reception** **Military Institute of Engineering - IME**

November 23 (Tuesday)

Session 1 **Ligand and Structure-Based Drug Design** Chair: Glaucius Oliva, Brazil	
9:00 – 9:15 am	Glaucius Oliva, Brazil **Overview and Introduction**
9:15 – 10:15 am	Eliezer J. Barreiro, Brazil **Design and Discovery of Novel Symbiotic Lead-Candidates**
10:15 – 11:15 am	Hugo Kubinyi, Germany **Virtual Screening: Problems and Success Stories**
11:15 – 11:30 am	**Coffee Break**
11:30 – 12:30 pm	Robert D. Clark, USA **Integrating Virtual HTS into Combinatorial Library Design**
12:30 – 1:30 pm	Osman F. Güner, USA **Effective Docking and Scoring: Novel Classification of Protein-Ligand Complexes based on Binding Sites Characteristics**
1:30 – 3:00 pm	**Lunch**
Session 2 **QSAR, ADME/Tox & Drug Design** Chair: Magaly Girão Albuquerque, Brazil	
3:00 – 3:15 pm	Magaly Girão Albuquerque, Brazil **Overview and Introduction**
3:15 – 4:15 pm	Yvonne C. Martin, USA **A Personal Viewpoint on the Computer Prediction of Biological Activity of Compounds**
4:15 – 5:15 pm	Christopher A. Lipinski, USA **Filters and Choices in Early Drug Discovery**
5:15 – 5:30 pm	**Coffee Break**
5:30 – 6:30 pm	Bernard Testa, Switzerland **Can Drug Metabolism be Predicted?**
6:30 – 7:30 pm	Anton J. Hopfinger, USA **The 4D-QSAR Paradigm: A General Tool for QSAR, Structure-Based Design and Molecular Similarity Applications**

November 24 (Wednesday)

Session 3 **Medicinal Chemistry of Organic Synthesis and Natural Products** Chair: Carlos A. Manssour Fraga, Brazil	
9:00 – 9:15 am	Carlos A. Manssour Fraga, Brazil **Overview and Introduction**
9:15 – 10:15 am	Barry M. Trost, USA **The Impact of New Synthetic Methodology on Strategies to Bioactive Targets**
10:15 – 10:30 am	**Coffee Break**
10:30 – 11:30 am	Rosendo A. Yunes, Brazil **Natural Products: New Perspectives in Medicinal Chemistry**
11:30 – 12:30 pm	Luiz Carlos Dias, Brazil **Approaches to the Stereoselective Synthesis of Biologically Active Natural Products**
12:30 – 2:00 pm	**Lunch**
Session 4 **Medicinal Chemistry: Sci-Mix** Chair: Carlos A. Montanari, Brazil	
2:15 – 2:30 pm	Carlos A. Montanari, Brazil **Overview and Introduction**
2:30 – 3:00 pm	Hugo Cerecetto, Uruguay ***N*-Oxide Containing Heterocycles as Trypanocidal drugs**
3:00 – 3:20 pm	Marcelo Santos Castilho, Brazil **Development of Enzyme Inhibitors as Potential Antiparasitic Agents**
3:20 – 3:40 pm	Marcelo Zaldini Hernandes, Brazil **An Initiative for 3D-QSAR Software Development: The CAMOL experience**
3:40 – 4:10 pm	Carlos Roque D. Correia, Brazil **Conformationally Restricted Glutamates. Total Enantioselective Synthesis of Highly Neuroexcitatory Acromelic Acid Analogues**
4:10 – 4:30 pm	**Coffee Break**
Poster Session I: 4:30 – 5:30 pm **Poster Session II: 5:30 – 6:30 pm** Chairs: Jose Daniel Figueroa Villar & Adriano D. Andricopulo, Brazil	

November 25 (Thursday)

Session 5 **Novel Approaches to Drug Discovery and Development** Chair: Richard C. Garratt, Brazil	
9:00 – 9:15 am	Richard C. Garratt, Brazil **Overview and Introduction**
9:15 – 10:15 am	Michael J. McLeish, USA **Development of Inhibitors of Phenylethanolamine *N*-methyltransferase as Potential Antihypertensives with an Unusual Mode of Action**
10:15 – 10:30 am	**Coffee Break**
10:30 – 11:30 am	Claudio Dalvit, Italy **Novel NMR Techniques for Efficient and Reliable High-Throughput Screening**
11:30 – 12:30 pm	Antonio Carlos Martins de Camargo, Brazil **EVASINs, New Antihypertensive Substances from Snake Venom**
Closing Remarks	
12:30 – 12:50 pm	Jose Daniel Figueroa Villar, Brazil

End of the Symposium