



The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

# PROGRAM

## THE 4<sup>th</sup> BRAZILIAN SYMPOSIUM ON MEDICINAL CHEMISTRY

### *SYSTEMS CHEMICAL BIOLOGY*

*Porto de Galinhas - PE*  
November 9-13, 2008

### SUNDAY, NOVEMBER 9, 2008

**PRE-  
SYMPOSIUM  
SHORT-  
COURSES**

(In Portuguese, pre-  
registration required)

November, 9

9 am–5 pm

**1. Medicinal chemistry: from genes to drugs**

Prof. Dr. Igor Polikarpov, São Carlos Physics Institute – Brazil  
and Dr. Andrei Leitão, University of New Mexico – USA

**2. Medicinal chemistry of anti-inflammatory drugs**

Prof. Dr. Fernando Cunha, University of Sao Paulo - Brazil

**3. Medicinal chemistry of antimalarials**

Prof. Dr. José Daniel Figueroa Villar, Military Institute of  
Engineering – Brazil

**4. Medicinal chemistry of trypanocide agents**

Prof. Dr. Julio A. Urbina, Venezuelan Institute for  
Scientific Research (Caracas, Venezuela) & Scientific  
Advisory Committee, Drugs for Neglected Diseases  
Initiative Geneva – Switzerland

Topics:

1. Pharmacological Effects and Targets
2. Biological Screening Assays
3. Structure-Activity Relationships

### Organizing Committee of the BrazMedChem2008

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP



The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

---

<b>2:00 – 6:00 pm</b>	<b>REGISTRATION</b>
<b>SUNDAY, NOVEMBER 9, 2008</b>	
<b>OPENING SESSION</b>	
7:00 – 7:30 pm	<b>Ivan da Rocha Pitta</b> , Federal University of Pernambuco, Brazil Welcome from the Symposium Chair
<b>OPENING CONFERENCE</b>	
7:30 – 8:30 pm	<b>Herbert Waldmann</b> Max-Planck-Institut für Molekulare Physiologie, Germany “ <b>Biology Oriented Synthesis</b> ”
8:30 – 10:00 pm	<b>WELCOME RECEPTION</b>

---

**Organizing Committee of the BrazMedChem2008**

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP



The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

---

<b>MONDAY, NOVEMBER 10, 2008</b>	
9:00 – 9:15 am	<b><u>SESSION 1</u></b>  <b><u>CHEMINFORMATICS AND SYSTEMS CHEMICAL BIOLOGY</u></b>  Chair: <b>Fernando Batista Da Costa</b> University of São Paulo, Brazil  Overview and Introduction
9:15 – 10:15 am	<b>Gabriele Cruciani</b> University of Perugia, Italy  “ <b>Milestones and Challenges in the Prediction of Human Metabolism</b> ”
<b>10:15 – 10:45 am</b>	<b>COFFEE BREAK</b>
10:45 – 11:45 am	<b>Tudor I. Oprea</b> University of New Mexico, USA  “ <b>Systems Chemical Biology: Integrating Chemistry and Biology for better Medicinal Chemistry</b> ”
11:45 am – 12:45 pm	<b>Andrew L. Hopkins</b> University of Dundee, UK (ex-Pfizer)  “ <b>Why Chemists Should be Promiscuous</b> ”
12:45 – 2:00 pm	<b>LUNCH</b>

---

**Organizing Committee of the BrazMedChem2008**

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP



The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

---

**MONDAY, NOVEMBER 10, 2008**

2:15 – 2:30 pm	<b><u>SESSION 2</u></b>  <b><u>LIBRARIES FOR SCREENING AND DRUG DESIGN</u></b>  Chair: <b>Vera Lúcia Eifler-Lima</b> Federal University of Rio Grande do Sul, Brazil  Overview and Introduction
2:30 – 3:30 pm	<b>Catrin Hasselgren</b> AstraZeneca R&D, Mölndal, Sweden  "Modelling and informatics support for safety and metabolism studies in early drug discovery projects"
3:30 – 4:30 pm	<b>Jean-Jacques Bourguignon</b> University of Strasbourg, France  "Screening of Compound Libraries for Drug Discovery: Overview of Screening Technologies, Structural Analysis of Libraries, Hit Selection and First Hit Optimization"
4:30 – 6:30 pm	<b>POSTER SESSION I. MARCELO ZALDINI AND MAGALY G. ALBUQUERQUE</b>
<b>6:30 PM</b>	<b>DINNER</b>

---

**Organizing Committee of the BrazMedChem2008**

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP



The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

---

<b>TUESDAY, NOVEMBER 11, 2008</b>	
9-12 am	<b>GROUP MEETING</b>
12-2 pm	<b>LUNCH</b>
2:00 - 2:15 pm	<b><u>SESSION 3</u></b>  <b><u>STRUCTURE AND ENERGETICS OF</u></b>  <b><u>DRUG-RECEPTOR INTERACTIONS</u></b>  Chair: <b>Carlos H. I. Ramos</b> State University of Campinas, Brazil  Overview and Introduction
2:15 - 3:15 pm	<b>John E. Ladbury</b> University College London, UK  <b>Application of Thermodynamic Parameters to Drug Design</b>
3:15 - 4:15 pm	<b>Glaucius Oliva</b> University of São Paulo, Brazil  <b>"Structural Bioinformatics and the Medicine of the Future"</b>
4:15 - 6:15 pm	<b>POSTER SESSION II. MARCELO ZALDINI AND MAGALY G. ALBUQUERQUE</b>
<b>6:15 PM</b>	<b>DINNER</b>

---

**Organizing Committee of the BrazMedChem2008**

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP



The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

---

<b>WEDNESDAY, NOVEMBER 12, 2008</b>	
9:00-9:15 am	<b><u>SESSION 4</u></b>  <b><u>STRATEGIES IN DRUG DESIGN</u></b>  Chair: <b>Adriano D. Andricopulo</b> University of São Paulo, Brazil  Overview and Introduction
9:15-10:15 am	<b>Michael H. Gelb</b> University of Washington, Seattle, USA  "Piggyback Medicinal Chemistry for the Development of Drugs for Malaria, African Sleeping Sickness and Chagas' Disease"
<b>10:15-10:45 am</b>	<b>COFFEE BREAK</b>
10:45-11:45 am	<b>Larry A. Sklar</b> University of New Mexico, USA  "HTS Flow Cytometry of Multiplexed Targets"
11:45-12:45 am	<b>John A. Tallarico</b> Novartis, USA  "Finding Targets for Drugs: The Chemical Genetic Approach"
<b>12:45-2 pm</b>	<b>LUNCH</b>

---

**Organizing Committee of the BrazMedChem2008**

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP



The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

---

<b>WEDNESDAY, NOVEMBER 12, 2008</b>	
2:00 – 2:15 pm	<b><u>SESSION 5</u></b>  <b><u>SYNTHESIS, DESIGN AND STRUCTURAL OPTIMIZATION</u></b>  Chair: <b>Arlene G. Corrêa</b> Federal University of São Carlos, Brazil  Overview and Introduction
2:15 – 3:15 pm	<b>Julio A. Urbina</b> Drugs for Neglected Diseases Initiative Geneva, Switzerland  <b>“Bisphosphonates as novel inhibitors of Trypanosoma cruzi hexokinase: quantitative structure-activity relationships, mechanism of action and physiological studies”</b>
3:15 – 4:15 pm	<b>Paulo Roberto Ribeiro Costa</b> Federal University of Rio de Janeiro, Brazil  <b>“From Naturally Occurring Pterocarpanes and Coumestans to New Prototypes for Anticancer, Antiparasitic and Antiophidic Therapy”</b>
<b>4:15 – 4:45 pm</b>	<b>COFFEE BREAK</b>

---

**Organizing Committee of the BrazMedChem2008**

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP



The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

---

<b>WEDNESDAY, NOVEMBER 12, 2008</b>	
4:45 pm	<b><u>SESSION 6</u></b>  <b><u>OPEN SCIENCE: MIX SESSION.</u></b> <b><u>POSTER INVITED SHORT LECTURES</u></b>  Chair: Tudor I. Oprea
4:45 – 5:05 pm	<b>Renato Ferreira de Freitas</b> , University of São Paulo, Brazil  "Discovering Novel Inhibitors of <i>Trypanosoma cruzi</i> GAPDH: A Virtual Screening, Calorimetric and Cell Assays"
5:05 – 5:25 pm	<b>Rodrigo Luiz Oliveira Rodrigues Cunha</b> , Federal University of São Paulo  "Telluranes: Promising Agents for Malaria Treatment as Revealed by a New Cell-based Assay"
5:25 – 5:45 pm	<b>Amanda Coelho Danuello</b> , State University of São Paulo, Brazil  "Molecular Modeling Studies of Semi-synthetic Piperidine anti-Alzheimer Prototypes"
5:45 – 6:05 pm	<b>Jerônimo Lameira Silva</b> , Federal University of Pará, Brazil  "Catalytic Mechanism Study of Human O-GlcNAcase by Molecular Dynamics and Quantum-Mechanical/Molecular-Mechanical"
6:05 – 6:25 pm	<b>Elisa Soares Leite</b> , Federal University of Pernambuco  "Docking of New Arylidene-Thiazolidinediones in the PPAR $\gamma$ Target"
<b>6:25 – 7:00 pm</b>	<b>Prize Awards Ceremony</b>
<b>8:30 – 12:00 pm</b>	<b>Gala Dinner (pre-registration required)</b>

---

**Organizing Committee of the BrazMedChem2008**

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP





The 4<sup>th</sup> Brazilian Symposium on Medicinal Chemistry  
Porto de Galinhas, Brazil, November 9-13, 2008  
<http://www.brazmedchem.iqsc.usp.br>  
[brazmedchem@iqsc.usp.br](mailto:brazmedchem@iqsc.usp.br)

---

<b>THURSDAY, NOVEMBER 13, 2008</b>	
9:00 – 9:15 am	<b><u>SESSION 7</u></b>  <b><u>THE ROLE OF NATURAL PRODUCTS IN DRUG DISCOVERY AND DEVELOPMENT</u></b>  Chair: <b>Isac Almeida de Medeiros</b> Federal University of Paraiba  Overview and Introduction
9:15 – 10:15 am	<b>Nicholas H. Oberlies</b> Research Triangle Institute International – USA  “ <b>Trekking for New Medicines: New Drug Leads from Under Explored Biodiversity</b> ”
10:15 – 10:30 am	<b>COFFEE-BREAK</b>
10:30 – 11:30 am	<b>Paulo Cezar Vieira</b> Federal University of São Carlos  “ <b>Natural Products and Drug Discovery</b> ”
11:30 am-12:30 pm	<b>Marilia O. F. Goulart</b> Federal University of Alagoas, Brazil  “ <b>Pharmacoelectrochemistry: a Tool for Discovery of Drugs and for the Investigation of Biological Mechanism of Action</b> ”
12:30 – 12:45 pm	<b>CLOSING REMARKS</b>  <b>Carlos A. Montanari</b> , University of São Paulo, Brazil
12:45 pm	<b>LUNCH</b>

---

**Organizing Committee of the BrazMedChem2008**

Chair: Ivan da Rocha Pitta, UFPE

Vice-Chair: Carlos Alberto Montanari, USP

Secretary General: Suely Lins Galdino, UFPE

Chair of the Scientific Committee: Fernando Queiroz Cunha, USP