

**11<sup>TH</sup> NUCLEAR MAGNETIC RESONANCE USERS MEETING**  
**WORKSHOP: NMR IN SOUTH AMERICA**  
**MAY 7<sup>th</sup> - 11<sup>th</sup>, 2007**  
**HOTEL DO FRADE, ANGRA DOS REIS, RJ, BRAZIL**

**GENERAL PROGRAM**

**MONDAY, MAY 7<sup>TH</sup>**

**05:30 PM – Opening Session**

Chairman: J.D. Figueroa Villar (Brazil), Presidente da AUREMN

In memory of the late Newton Flavio B. dos Santos

Chair: Alvicler Magalhães (Brazil)

**06:00 PM – Opening Lecture**

*Protein structure determination by MAS solid-state NMR: application to fibrils and membrane proteins*

Lecturer: Hartmut Oschkinat (Germany)

Chair: José Ricardo M. Pires (Brazil)

**07:00 PM – Cocktail and Dinner**

BOOK LAUNCH

“FUNDAMENTOS E APLICAÇÕES DA RESSONÂNCIA MAGNÉTICA NUCLEAR (N. 3)  
*Introdução à Ressonância Paramagnética de Onda Contínua. Aplicações ao Estudo de Complexos de Metais de Transição*”

Ney Vernon Vugman (UFRJ) e Marcelo H. Herbst (UFRRJ)

**TUESDAY, MAY 8<sup>TH</sup>**

**08:30 AM – Seminar (Portuguese)**

Sonia M. C. Menezes (Brazil)

**09:00 AM – Plenary Lecture**

*Characterization of polyatomic structural motifs in crystalline and disordered inorganic solids using Solid State NMR*

Lecturer: Franck Fayon (France)

Chair: Rosane A.S. San Gil (Brazil)

**09:45 AM – COFFE-BREAK**

**10:15 AM – Oral Communications (4)**

Chair: Fábio Almeida (Brazil)

*Conformational Effects on Polycyclic Half-Cage Alcohols by Natural Chemical Shielding Analysis*

Peter Rudolf Seidl, Jacques Fernandes Dias, José Walkimar de Mesquita Carneiro, José Glauco Ribeiro Tostes, Andréas Koch, Erich Kleinpeter

*Structural Studies of Thioredoxins 1 and 2 from Saccharomyces Cerevisiae During the Interaction with their Cellular Targets*

Gisele Cardoso de Amorim, Anderson de Sá Pinheiro, Luis Eduardo Soares Netto, Ana Paula Valente and Fábio Ceneviva Lacerda de Almeida.

*Analysis of Phylloseptin Peptides in Membranes: Helix Tilt & Rotational Pitch Angles from Combined 15N & 2H Solid-State NMR*

Jarbas Magalhães Resende, Cléria Mendonça Moraes, Amary César, Philippe Bertani, Dorila Piló-Veloso, and Burkhard Bechinger

*Quantum State Tomography For General Quadrupolar Systems: Theory And Applications*

João Teles, Ruben Aucçaise, Eduardo R. deAzevedo, Roberto Sarthour, Ivan S. Oliveira, Tito J. Bonagamba

**11:30 AM – Vendor Conference 1 – VARIAN**

Chair: José Dias de Souza Filho (Brazil)

**12:00 PM – LUNCH**

**03:00 PM – Session State-of-the-art in NMR I**

Chair: Roberto Rittner (Brazil)

**Participants**

*NMR-based Structural Genomics and Ligand Discovery*

Hartmut Oschkinat (Germany)

*Advanced Dipolar NMR Techniques for Structural Studies of Disordered Materials*

Helmut Eckert (Germany)

*Ab Initio Calculation of NMR Properties ( $\delta$ , J, Anisotropic, Electronic and Steric Substituent Effects) of Small Organic Molecules*

Erich Kleinpeter (Germany)

**04:30 PM – COFFEE-BREAK**

**05:00 PM – Session State-of-the-art in NMR II**

Chair: Eduardo Ribeiro Azevedo (Brazil)

**Participants**

*Mouse and Art*

Bernhard Blümich (Germany)

*A Selective H-F NOESY Experiment*

Bruce Adams (USA)

*Accurate Heteronuclear J-Coupling Measurements in Dilute Spin Systems using the multiple-quantum filtered J-resolved experiment*

Franck Fayon (France)

**06:30 PM – Vendor Conference 2 – TEDIABRAZIL/WILMAD**

Chair: Carlos R. Kaiser (Brazil)

**07:00 PM - DINNER**

**09:00 PM – Poster Session I**

Chair: Rosana Garrido (Brazil)

## WEDNESDAY, MAY 9<sup>TH</sup>

**08:30 AM – Seminar** (Portuguese)  
Claudia Jorge do Nascimento (Brazil)

**09:00 AM – Plenary Lecture**  
*Broadband F19 Pulse Sequences*  
Lecturer: Bruce Adams (USA)  
Chair: Anita J. Marsaioli (Brazil)

**09:45 AM – COFFEE BREAK**

**10:15 AM – Seminar** (Portuguese)  
Peter R. Seidl (Brazil)

**10:45 AM – Plenary Lecture**  
*Visualization of Aromaticity and Antiaromaticity by Through Space NMR Shieldings*  
Lecturer: Erich Kleinpeter (Germany)  
Chair: Claudio Tormena (Brazil)

**11:30 AM – Vendor Conference 3 – BRUKER**  
Chair: Edilberto R. Silveira (Brazil)

**12:00 PM – LUNCH**

**03:00 PM – Seminar** (Portuguese)  
Rodrigo Bagueira (Brazil)

**03:30 PM – Plenary Lecture** (English)  
*Mobile NMR: Materials and Function*  
Lecturer: Bernhard Blümich (Germany)  
Chair: Naira M.S. Ruiz (Brazil)

**04:30 PM – COFFEE-BREAK**

**05:00 PM – AUREMN General Assembly**

**Opening: José Daniel Figueroa Villar (IME), President of AUREMN**

Sonia Maria Cabral de Menezes (PETROBRAS), Vice-President

Luzineide Wanderley Tinoco (UFRJ), Secretary

Rosane Aguiar da Silva San Gil (UFRJ), Treasurer

**New Members Commission:**

Naira Machado da Silva Ruiz (PUC-RIO)

**Informatics and Statistic Commission**

Kátia Zaccur Leal (UFF)

Naira Machado da Silva Ruiz (PUC-RIO)

**Editorial Office**

José Daniel Figueroa Villar (IME)

Maria Inês Bruno Tavares (IMA-UFRJ)

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**Library Commission**

Eduardo Miguez Bastos da Silva (IMA-UFRJ)

**Nomenclature Commission**

Rosana Garrido Gomes (PUC)

**Courses Commission**

Camila Bastos de Oliveira Mansur (NPPN-UFRJ)

**General Topics**

**07:00 PM – DINNER**

**09:00 PM – Poster Session II**  
Chair: Ivan P. A. Campos (Brazil)

## THURSDAY, MAY 10<sup>TH</sup>

### 08:30 AM – Lectures

Chair: Maria Inês B. Tavares (Brazil)

*Food NMR application*

Lecturer: Antonio G. Ferreira (Brazil)

*Metal Ions in Synucleinopathies: an Spectroscopic View*

Lecturer: Claudio R. Fernandez (Argentina)

*Investigation of the Three-Dimensional Structures of Zeolite Molecular Sieves With Sorbed Organic Guest Molecules by High Resolution Solid State NMR*

Lecturer: Anix Diaz (Venezuela)

### 09:45 AM – COFFE BREAK

### 10:15 AM – Lectures

Chair.: Nilo Zanatta (Brazil)

*NMR and Theoretical Studies on the Complexation of Anionic Guests with Cyclodextrins*

Lecturer: Joel Alderete (Chile)

*Novel structural and thermodynamic insights on dengue virus fusion*

Lecturer: Ronaldo Borges (Brazil)

*Spin-spin Coupling Constants and Intra-Molecular Interactions*

Lecturer: Ruben Contreras (Argentina)

### 12:00 PM – LUNCH

### 03:00 PM – Lectures

Chair: Luiz A. Colnago (Brazil)

*NMR Studies of Electron-Transfer Copper Proteins*

Lecturer: Alejandro Vila (Argentina)

*PLS Correlation between Refined Product Yields and Physicochemical Properties with the 1-H NMR Spectra of Colombian Crude Oils*

Lecturer: Daniel Molina (Colombia)

*Mode of Action of New Anti Parasite Agents. <sup>1</sup>H NMR Studies*

Lecturer: Hugo Cerecetto (Uruguay)

*Formation of Ionic Clusters and Reaction Intermediate*

Lecturer: Fernando Hallwass (Brazil)

### 04:30 PM – COFFE-BREAK

### 05:00 PM – Round Table: NMR in South America

Chair: Peter R. Seidl (Brazil)

#### Participants

Alejandro Vija (Argentina)

Anix Diaz, (Venezuela)

Antonio G. Ferreira (Brazil)

Ruben Contreras (Argentina)

Daniel Molina (Colombia)

Hugo Cerecetto (Uruguay)

Joel Alderete (Chile)

### 07:00 PM - DINNER

## **FRIDAY, MAY 11<sup>TH</sup>**

### **08:30 AM – Evaluation Session**

Chair: Kátia Zaccur Leal (Brazil)

### **09:00 AM – Closing Session**

José Daniel Figueroa Villar (Brazil)

### **10:00 AM – Social Program**

### **12:00 PM – LUNCH**

### **03:00 PM – Trip Back to Rio de Janeiro**

(Arrival to Rio de Janeiro International Airport at 06:00PM)