

12TH NUCLEAR MAGNETIC RESONANCE USERS MEETING
3RD IBEROAMERICAN NMR MEETING
MAY 4TH TO 08TH, 2009 - HOTEL DO FRADE, ANGRA DOS REIS, RJ, BRAZIL

PROGRAM

MONDAY, MAY 4TH

05:00 PM – Opening Session

AUREMN's President: José Daniel Figueroa Villar (IME/RJ, Brazil)

05:30 PM – Opening Lecture

ATOMIC-RESOLUTION STRUCTURES OF MICROCRYSTALS, AMYLOIDS AND PRIONS BY SOLID-STATE NMR

Lecturer: Beat H. Meier (ETH Zurich, Switzerland)

Chair: Sonia Maria Cabral de Menezes (PETROBRAS/CENPES, Brazil)

06:30 PM – Plenary Lecture

GEOMETRICAL STRUCTURE, ELECTRONIC STRUCTURE, AND STRUCTURAL DYNAMICS OF BIOLOGICAL AND SYNTHETIC MACROMOLECULES AS SEEN BY EPR SPECTROSCOPY

Lecturer: Gunnar Jeschke (ETH Zurich, Switzerland)

Chair: Antonio J. Costa Filho (USP/SC, Brazil)

07:30 PM – COCKTAIL

BOOK LAUNCH

“FUNDAMENTOS E APLICAÇÕES DA RESSONÂNCIA MAGNÉTICA NUCLEAR. DIFUSÃO MOLECULAR POR RMN” - (N. 4, 1^a. EDIÇÃO)

Authors: Anita Jocelyne Marsaioli (UNICAMP), Antonio Laverde Jr. (UNICAMP), Fred Yukio Fujiwara (UNICAMP), Isis Martins Figueiredo (UNICAMP), Sergio Antonio Fernandes (UNICAMP), Antonio Gilberto Ferreira (UFSCar), Lucinéia Vizzotto (UFSCar), Alexandre Araújo de Souza (UFPI)

BOOK LAUNCH

“FUNDAMENTOS E APLICAÇÕES DA RESSONÂNCIA MAGNÉTICA NUCLEAR. ASPECTOS QUÂNTICOS DA RESSONÂNCIA MAGNÉTICA NUCLEAR” - (N. 2, 3^a. EDIÇÃO)

Author: José Daniel Figueroa Villar (IME/RJ)

08:30 PM – DINNER

TUESDAY, MAY 5TH

08:30 AM – Seminar (Portuguese)
Luzineide W. Tinoco (UFRJ, Brazil)

09:00 AM – Plenary Lecture
FINDING A NEEDLE IN A HAYSTACK: PHARMACEUTICAL AND BIOCHEMICAL MICROANALYSIS USING MICROCOIL NMR
Lecturer: Cynthia Larive (University of California, USA)
Chair: Anita Marsaioli (UNICAMP, Brazil)

09:50 AM – COFFEE-BREAK

10:20 AM – Conference
NEW DEVELOPMENTS IN HIGH-RESOLUTION ¹H SOLID-STATE NMR AT HIGH FIELD AND VERY-FAST MAS
Lecturer: Luis Mafra (University of Aveiro, Portugal)
Chair: Teresa Blasco (UPV, Spain)

11:00 AM – Conference
NEW INSIGHTS INTO HUMAN RIBONUCLEASES: STRUCTURE, DYNAMICS AND STABILITY OF RNASE 1 AND RNASE 3 STUDIED BY NMR
Lecturer: Marta Bruix (IQFR, CSIC, Spain)
Chair: Dorila P. Veloso (UFMG, Brazil)

11:40 AM – Vendor Conference 1 – ANASAZI
APPLICATIONS OF NMR FOR THE STUDY OF FOODS AND CONSUMER PRODUCTS TO CREATE INTEREST FOR NON-SCIENCE MAJORS
Lecturer: Donald Bouchard (ANASAZI Instruments, USA)

12:30 PM – LUNCH

03:30 PM – Mini-Conference
TOWARDS THE OPTIMIZATION OF TARGETED CONTRAST AGENTS FOR MRI-BASED MOLECULAR IMAGING APPLICATIONS
Lecturer: Carlos F.G.C. Geraldés (University of Coimbra, Portugal)
Chair: João Batista Fernandes (UFSCar, Brazil)

04:00 PM – Oral Communications I
Chair: João Batista Fernandes (UFSCar, Brazil)

STRUCTURE OF Art v 1 AND DYNAMICS OF IgE INTERACTION BY NMR: AN APPROACH TO DEVELOP HYPOALLERGEN VACCINE
Guilherme Razzera; Gabriele Gadermaier; Marcius S. Almeida; Fátima Ferreira; Fábio C.L. Almeida and Ana Paula Valente

METODOLOGY TO MEASURE THERMAL DIFFUSIVITY IN INTACT SEED IN SOIL COLUMN BY LOW RESOLUTION NMR
Maria G. A. Carosio; Luis A. Colnago

CHARACTERIZATION OF INTRINSICALLY DISORDERED PROTEINS BY NMR: THE CASE OF α -SYNUCLEIN
María L. Orcellet, Gonzalo R. Lamberto, Andrés Binolfi, Carlos W. Bertoncini, Markus Zweckstetter, Christian Griesinger and Claudio O. Fernández

05:00 PM – COFFEE-BREAK

05:30 PM – Poster Session I (ODD NUMBER)
Chair: Anderson Barison (UFPR, Brazil)

08:00 PM - DINNER

WEDNESDAY, MAY 6TH

08:30 AM – Seminar (Portuguese)
Fabio C.L. Almeida (UFRJ, Brazil)

09:00 AM – Plenary Lecture
OPTIMAL CONTROL OF SPIN DYNAMICS IN MAGNETIC RESONANCE
Lecturer: Steffen J. Glaser (Technical University of Munich, Germany)
Chair: Claudia J. Nascimento (UNB, Brazil)

09:50 AM – COFFEE-BREAK

10:20 AM – Conference
MMR OF ORGANOMETALLIC COMPOUNDS: MULTINUCLEAR, MAGIC OR MASOCHIST MAGNETIC RESONANCE TO UNRAVEL THE POTION?
Lecturer: Fernando López Ortiz (University of Almeria, Spain)
Chair: Teresa Nunes (UTL, Portugal)

11:00 AM – Conference
THE NOVEL VirB7 COMPONENT OF THE XANTHOMONAS TYPE IV SECRETION SYSTEM COMBINES A CANONICAL VirB7 MOTIF WITH A PERIPLASMATIC SIGNALING DOMAIN
Lecturer: Chuck S. Farah (USP, Brazil)
Chair: Alejandro Vila (University of Rosario, Argentina)

11:40 AM – Vendor Conference 2 – BRUKER
(AUTOMATED) STRUCTURE ELUCIDATION
Lecturer: Rainer Kerssebaum (Bruker BioSpin, Germany)

12:30 PM – LUNCH

03:30 PM – Mini-Conference
FAST SCREENING AND STRUCTURAL CHARACTERIZATION OF MULTIDOMAIN PROTEINS
Lecturer: Rodolfo Rasia (University of Rosario, Argentina)
Chair: Antonio Donaire (University of Murcia, Spain)

04:00 PM – Oral Communications II
Chair: Antonio Donaire (University of Murcia, Spain)

INTERMEDIATE MOTIONS AS STUDIED BY LEE-GOLDBURG CROSS-POLARIZATION NMR
Marcio Fernando Cobo, Katerina Malinakowa, Detlef Reichert, Kay Saalwächter and Eduardo Ribeiro de Azevedo

¹H NMR SPECTROSCOPY AND CHEMOMETRICS IN METABOLIC PROFILING OF HUMAN BLOOD SERUM FOR IDENTIFICATION OF BIPOLAR DISORDER BIOMARKERS
Alessandra Prando, Alessandra Sussulini, Danilo A. Maretto, Ronei J. Poppi, Cláudio E. M. Banzato, Marco A. Z. Arruda and Ljubica Tasic

REVEALING THE GLOBAL MECHANISM OF INTERACTION OF CtCBM11
Aldino Viegas, Anjos L. Macedo, Maria João Romão, Carlos Fontes, Ana Luísa Carvalho, Eurico J. Cabrita

05:00 PM – COFFEE-BREAK

05:30 PM – Poster Session II (EVEN NUMBER)
Chair: Rosane Aguiar da Silva San Gil (UFRJ, Brazil)

08:00 PM - DINNER

THURSDAY, MAY 07TH

08:30 AM – Seminar (Portuguese)
Ana Carolina Zeri (LNLS, Brazil)

09:00 AM – Plenary Lecture
THE CHOREOGRAPHY OF AN ENZYME'S DANCE
Lecturer: Dorothee Kern (Brandeis University, USA)
Chair: Ana Paula Valente (UFRJ, Brazil)

09:50 AM – COFFEE-BREAK

10:20 AM – Conference
HIGH-THROUGHPUT, NON-DESTRUCTIVE DETERMINATION OF QUALITY OF AGRICULTURAL PRODUCTS BY NMR
Lecturer: Luiz Alberto Colnago (EMBRAPA, Brazil)
Chair: Fabio Bonk (UNICAMP, Brazil)

11:00 AM – Conference
NMR SPECTROSCOPY - A USEFUL TOOL TO ELUCIDATE THE PHARMACOLOGICAL ROLE OF Li^+ IN BIPOLAR DISORDER
Lecturer: M. Margarida Castro (University of Coimbra, Portugal)
Chair: Ernani Abicht Basso (UEM, Brazil)

11:40 AM – Vendor Conference 3 – VARIAN
VARIAN MR SYSTEMS - LATEST TECHNOLOGIES
Lecturer: Thomas Gottschalk (Varian INC., USA)

12:30 PM – LUNCH

03:30 PM – Mini-Conference
THE INTRINSICALLY UNFOLDED UNIQUE DOMAIN OF c-Src: STRUCTURE, INTERACTIONS AND PHOSPHORYLATION STUDIED BY NMR
Lecturer: Miquel Pons (University of Barcelona, Spain)
Chair: Eurico Cabrita (UNL, Portugal)

04:00 PM – Oral Communications III
Chair: Eurico Cabrita (UNL, Portugal)

¹³C-NMR SIGNAL ENHANCEMENT BY USING PARAHYDROGEN INDUCED POLARIZATION (PHIP) AND APPROPRIATE PULSE SEQUENCES

Meike Roth, Rodolfo Acosta, Joachim Bargon, Hans W. Spiess, Achim Koch, Kerstin Münnemann

INTERACTION STUDIES OF PHOSPHORYLATED N-TERMINAL PEPTIDE OF MARCKS PROTEIN AND THE MONOCLONAL ANTIBODY 3C3: NMR AND CIRCULAR DICHROISM STUDIES

Anobom, C. D.; Fraga J. L.; Zolessi F. R., Arruti C., Tinoco L. W.

¹H NMR SATURATION TRANSFER INTERACTIONS MAPPING BETWEEN ACETYLCHOLINESTERASE AND AMARYLLIS ALKALOIDS

Anita J. Marsaioli, Lucas G. Martins, Raquel M. Braga, Maria do Socorro S. Silva, Roberto Rittner, Cleverton C. Bocca

05:00 PM – COFFEE-BREAK

05:30 PM – AUREMN General Assembly

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

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

Luzineide Wanderley Tinoco (NPPN-UFRJ), Secretary

Rosane Aguiar da Silva San Gil (IQ-UFRJ), Treasurer

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Nomenclature Commission

Rosana Garrido Gomes (PUC-R)

Courses Commission

Claudia Nascimento (UNB)

General Topics

The Liquid Helium Crisis (White Martins/Praxair)

08:00 PM - DINNER

FRIDAY, MAY 08TH

08:30 AM – Evaluation Session

Chair: Simone Gonçalves (UFPE, Brazil)

09:30 AM – Closing Session

José Daniel Figueroa Villar, Chairman (IME/RJ, Brazil)

10:00 AM – Social Program

12:00 PM – LUNCH

03:00 PM – Return to Rio de Janeiro

(Arrival to Rio de Janeiro International Airport approximately at 06:00PM and Domestic Airport approximately at 07:00PM)

POSTERS

Tr 01 – ¹H NMR SATURATION TRANSFER INTERACTIONS MAPPING BETWEEN ACETYLCHOLINESTERASE AND AMARYLLIS ALKALOIDS

Anita J. Marsaioli, Lucas G. Martins, Raquel M. Braga, Maria do Socorro S. Silva, Roberto Rittner and Cleverson C. Bocca*

Tr 02 – ¹H NMR SPECTROSCOPY AND CHEMOMETRICS IN METABOLIC PROFILING OF HUMAN BLOOD SERUM FOR IDENTIFICATION OF BIPOLAR DISORDER BIOMARKER

*Alessandra Prando, Alessandra Sussulini, Danilo A. Mareto, Ronei J. Poppi, Cláudio E. M. Banzato, Marco A. Z. Arruda and Ljubica Tasic**

- Tr 03 – **$^1J_{CF}$ COUPLING CONSTANT THEORETICAL AND EXPERIMENTAL STUDY OF FLUOROBENZENE AND DERIVATIVES**
*Janaina D. Vilcachagua**, Lucas C. Ducati, Gabriela F. Pereira, Cláudio F. Tormena and Roberto Rittner
- Tr 04 – **^{13}C -NMR SIGNAL ENHANCEMENT BY USING PARAHYDROGEN INDUCED POLARIZATION (PHIP) AND APPROPRIATE PULSE SEQUENCES**
*Meike Roth**, Rodolfo Acosta, Joachim Bargon, Hans W. Spiess, Achim Koch and Kerstin Münnemann
- Tr 05 – **^{31}P MAS NMR AS A TOOL TO EVALUATE THE EFFECT OF SOYBEAN OIL ON HYDROTREATMENT CATALYST**
*Sonia C. Menezes**, Naira Ruiz, Cristina Cavalcanti, Marcelo Pacheco, Jefferson Gomes, Raissa M. Silva, José Luiz Zotin and Cláudia Chaves
- Tr 06 – **A PROGRAM FOR THE SIMPLE ANALYSIS OF MIXTURES BY NMR: APPLICATION TO METABOLOMIC DATA FROM STUDIES OF TOMATO RIPENING**
*Luciano A. Abriata**, Augusto Sorrequieta and Estela Valle
- Tr 07 – **ACID SITES IN SILICOALUMINOPHOSPHATE CAL-2 PROBED BY MULTINUCLEAR MAGNETIC RESONANCE**
*Fábio A. Bonk**, Darlene Felix, Erica C. O. Munsignatti and Heloise O. Pastore
- Tr 08 – **ADVANCED SSNMR TECHNIQUES, FTIR AND XRD APPLIED TO POLYMORPHISM IN A PHARMACEUTICAL COMPOUND**
*Yamila Garro Linck**, Ana K. Chattah, Carolina B. Romañuk, María E. Olivera, R. Baggio, M. T. Garland, Silvia L. Cuffini, Rubén H. Manzo and Gustavo A. Monti
- Tr 09 – **ANALYSIS OF RELAXATION TIMES IN FLOW CWFP-NMR**
*Antonio Marchi Netto** and Luiz Alberto Colnago
- Tr 10 – **BEAN CROPS DISCRIMINATION ACCORDING TO TRANSGENIC AND CONVENTIONAL ORIGIN BY 1H HR-MAS NMR AND CHEMOMETRIC ANALYSIS**
Rafael Choze, Pedro Paulo Araujo Cavalcante, Glaucia Braz Alcantara, Josias Corrêa de Faria and Luciano Morais Lião
- Tr 11 – **BOVINE METABOLOMICS: A NMR APPROACH**
*Matheus P. Postigo**, Ana Carolina de Souza Chagas, Márcia Cristina de Sena Oliveira and Luiz Alberto Colnago
- Tr 12 – **CHARACTERIZATION OF INTRINSICALLY DISORDERED PROTEINS BY NMR: THE CASE OF α -SYNUCLEIN**
*María L. Orcellet**, Gonzalo R. Lamberto, Andrés Binolfi, Carlos W. Bertoncini, Markus Zweckstetter, Christian Griesinger and Claudio O. Fernández

- Tr 13 – **CHARACTERIZATION OF POLYSACCHARIDES FROM *Maytenus ilicifolia* BY LOW FIELD NUCLEAR MAGNETIC RESONANCE**
Mônica Santos de Moura Preto and Maria Inês Bruno Tavares*
- Tr 14 – **CHEMOMETRIC ANALYSIS APPLIED TO ^1H , ^1H HR-MAS NMR AND FT-IR DATA FOR QUALITY ASSESSMENT OF THE PHYTOMEDICINE “GINSENG BRASILEIRO”**
Katyúscya Veloso Leão, Márcia M. C. Ferreira, Glyn M. Figueira³ and Antonio G. Ferreira*
- Tr 15 – **COMBINING SOLUTION AND SOLID STATE ^1H AND ^{13}C NMR TO CHARACTERIZE PVC SUBSTITUTED WITH ALKYL GROUPS**
*Maria dos Prazeres A. Silva and Rosa Maria Souto-Maior**
- Tr 16 – **COMPLETE ^1H AND ^{13}C NMR DATA ASSIGNMENT FOR A NEW SEMI-SYNTHETIC FURANOHELIANGOLIDE**
Daiane C. Sass, Vladimir C. G. Heleno, João L. C. Lopes and Mauricio G. Constantino*
- Tr 17 – ***Cucumis melo* L (MELON) SEED OIL CHARACTERIZATION BY ^1H NMR**
*Eliane May de Lima and Paulo Irajara Borba Carneiro**
- Tr 18 – **CULTIVARS DISCRIMINATION BY ^1H NMR (HR-MAS AND IN SOLUTION) AND CHEMOMETRIC ANALYSIS APPLIED TO SUGARCANE LEAVES**
*Elenilson de G. Alves Filho, Lorena Mara A. e Silva, Luciano Morais Lião and Glaucia Braz Alcantara**
- Tr 19 – **CWFP AS A TOOL FOR MONITORING THE CURE OF A COMMERCIAL EPOXY RESIN IN LOW FIELD NMR**
Tiago Venâncio and Luiz Alberto Colnago*
- Tr 20 – **DETERMINATION OF TOTAL GLYCERIN IN BIODIESEL USING ^1H NMR WITH MULTIVARIATE DATA ANALYSIS**
Francisco F. Gambarra-Neto, Marcos R. Monteiro and Antonio Gilberto Ferreira*
- Tr 21 – **ELECTRON PARAMAGNETIC RESONANCE STUDIES AT X- AND Q-BAND OF THE DINUCLEAR COMPOUND $[\text{Cu}(\text{flu})_2\text{DMF}]_2$**
*Lia M. B. Napolitano and Otaciro R. Nascimento**
- Tr 22 – **ELECTRONIC STRUCTURE OF CUA SITES EXPLORED BY NMR SPECTROSCOPY**
*Luciano A. Abriata, Gabriela N. Ledesma and Alejandro J. Vila**
- Tr 23 – **EXPERIMENTAL AND THEORETICAL STUDY OF $^1J_{\text{CH}}$ SCALAR COUPLINGS TRENDS IN 1,3-DITHIANES**
Gisele F. Gauze, Ernani A. Basso and Cláudio F. Tormena*

- Tr 24 – **EXPERIMENTAL AND THEORETICAL STUDY OF CAGE-LIKE COMPOUNDS: UNAMBIGUOUS ASSIGNMENT OF NMR SIGNALS**
*Valdemar Lacerda Jr. *, Roberta C. Salles, Ronaldo Scarpate, Adilson Beatriz, Felicia M. Ito, Reginaldo B. dos Santos, Sandro J. Greco and Eustaquio V. R. de Castro*
- Tr 25 – **EXPERIMENTAL AND THEORETICAL STUDY ON NMR $^1J_{CH}$, $^1J_{CF}$ AND $^2J_{CF}$ SCALAR COUPLINGS IN 4-*TERT*-BUTYL-2-FLUORO-CYCLOHEXANOL ISOMERS**
Pedro R. Anizelli and Cláudio Francisco Tormena*
- Tr 26 – **FLUID QUANTIFICATION IN CRUDE OIL–WATER BIPHASIC MIXTURES BY LOW-FIELD NMR**
Renzo C. Silva, Giovanna F. Carneiro, Tiago Venâncio, Jair C. C. Freitas, Valdemar Lacerda Júnior and Eustáquio V. R. de Castro*
- Tr 27 – **FOSFOMYCIN BINDING EVENTS IN LIVING BACTERIAL CELLS OBSERVED BY NMR SPECTROSCOPY**
*Lucas G. Martins, Cíntia D. F. Milagre, Luís F. Cabeça and Anita J. Marsaioli**
- Tr 28 – **HOOKE’S “LAPACHOL PEROXIDE” REVISITED¹**
Eufrânio N. da Silva Júnior, Maria C.F.R. Pinto, Kelly C.G. de Moura, Carlos A. de Simone, Claudia J. Nascimento, Carlos Kleber Z. Andrade and Antônio V. Pinto*
- Tr 29 – **HOW WELL DOES NMR BEHAVE IN NATURAL PRODUCTS STRUCTURE DETERMINATION? A SURVEY OF NATURAL PRODUCTS PUBLISHED 2007 AND 2008.**
*Erika Martins de Carvalho, Fernanda Antonia Pereira and Jochen Junker**
- Tr 30 – **HR-MAS NMR AND MULTIVARIATE ANALYSIS OF METABOLIC CHANGES ASSOCIATED TO TOMATE RIPENING: EFFECT OF TOMATO VARIETY**
María José Iglesias, Estela M. Sánchez and Fernando López Ortiz*
- Tr 31 – **IMPROVEMENTS IN THE CWFP METHOD FOR SOLVENT SUPPRESSION IN HIGH RESOLUTION NMR**
Tiago Venâncio and Luiz Alberto Colnago*
- Tr 32 – **INSTRUMENTAL ASPECTS TO IMPLEMENTING SOLID STATE NMR TECHNIQS HETCOR AND MQHETCOR**
Fábio A. Bonk, Alvicler Magalhães, Darlene Felix and Heloise O. Pastore*
- Tr 33 – **INTERACTION STUDIES OF PHOSPHORYLATED N-TERMINAL PEPTIDE OF MARCKS PROTEIN AND THE MONOCLONAL ANTIBODY 3C3: NMR AND CIRCULAR DICHROISM STUDIES**
Anobom, C. D, Fraga J. L., Zolessi F. R., Arruti C. and Tinoco L. W*

- Tr 34 – **INTERMEDIATE MOTIONS AS STUDIED BY LEE-GOLDBURG CROSS-POLARIZATION NMR**
*Marcio Fernando Cobo**, *Katerina Malinakowa*, *Detlef Reichert*, *Kay Saalwächter* and *Eduardo Ribeiro deAzevedo*
- Tr 35 – **IS THIS REALLY A CARBONYL ¹³C NMR SIGNAL?**
*Edilene D. Rodrigues**, *Denise B. da Silva*, *Dionéia C. R. de Oliveira* and *Gil V. J. da Silva*
- Tr 36 – **ISOLATION, CHARACTERISATION, AND NMR STUDY OF PECTINS FROM *Citrus Aurantium* (LARANJA AZEDA).**
Fernando V. Maluf, *Paulo Irajara Borba Carneiro **, *Carmen L. O. Petkowicz* and *Eliana Beleski B. Carneiro*
- Tr 37 – **LOSCHMIDT ECHO AS INDICATOR OF DECOHERENCE IN MANY BODY SPIN SYSTEMS**
*Claudia. M. Sánchez**, *Patricia R. Levstein*, *Rodolfo H. Acosta* and *Ana K. Chattah*
- Tr 38 – **LOW AND HIGH FIELD NMR STUDY OF MONGUBA (*Pachira aquatica* Aubl.) OIL**
*Giovanna F. Carneiro**, *Manuela C. Brum*, *Luna S. dos Santos*, *Renzo C. Silva*, *Tiago Venâncio*, *Jair C. C. Freitas*, *Reginaldo B. dos Santos*, *Valdemar Lacerda Jr.* and *Eustáquio V. R. de Castro*
- Tr 39 – **LOW-FIELD ¹H NMR STUDY OF PLASMA TREATED HEAVY OILS**
*Hercílio D. A. Honorato**, *Renzo C. Silva*, *Cleiton K. Piumbini*, *Jair C. C. Freitas*, *Alfredo G. Cunha*, *Francisco G. Emmerich*, *Valdemar Lacerda Júnior* and *Eustáquio V. R. de Castro*
- Tr 40 – **MEMBRANE INTERACTION AND STRUCTURAL CHARACTERIZATION OF SEVERAL PUTATIVE FUSION PEPTIDES FROM VSV G PROTEIN**
*Carolina Galvão Sarzedas**, *Nathalia Oliveira*, *Fabiana Avila Carneiro*, *Catarina A. Miyamoto*, *Ana Paula Valente*, *Andrea Thompson Da Poian* and *Fábio C.L. Almeida*
- Tr 41 – **MEMBRANE STRUCTURE AND CONFORMATIONAL CHANGES DURING BILAYER-ASSOCIATION OF THE ANTIBIOTIC HETERODIMERIC PEPTIDE DISTINCTIN BY ORIENTED SOLID-STATE NMR SPECTROSCOPY**
*Jarbas M. Resende**, *Victor H. O. Munhoz*, *Christopher Aisenbrey*, *Cléria M. Moraes*, *Rodrigo Verly*, *Philippe Bertani*, *Amary Cesar*, *Dorila Piló-Veloso* and *Burkhard Bechinger*
- Tr 42 – **METABOLIC PROFILE AND IDENTIFICATION OF NITAZOXANIDE DRUG METABOLITE IN HUMAN URINE BY ¹H NMR SPECTROSCOPY**
*Eduardo S. P. Nascimento**, *Elisangela F. Boffo* and *Antonio G. Ferreira*

- Tr 43 – **METABONOMICS: HEPATITIS C URINALYSIS BY ¹H NMR TO DISTINGUISH BETWEEN HCV POSITIVE AND NEGATIVE PATIENTS**
*Ricardo O. Silva**, Michele M. G. Godoy, Edmundo P. A. Lopes, Simone M. C. Gonçalves, Fernando Hallwass and Alfredo M. Simas
- Tr 44 – **METODOLOGY TO MEASURE THERMAL DIFFUSIVITY IN INTACT SEED IN SOIL COLUMN BY LOW RESOLUTION NMR**
*Maria G. A. Carosio** and Luis A. Colnago
- Tr 45 – **MODELL-FREE DETECTION OF MILLISECOND MOTION IN SOLID PROTEINS: DIPOLAR CODEX WITH SITE-SPECIFIC RESOLUTION**
*Alexey Krushelnitsky, Eduardo Ribeiro deAzevedo, Kay Saalwächter, Bernd Reif, Veniamin Chevelkov and Detlef Reichert **
- Tr 46 – **MONITORING THE SEPARATION OF REPRESENTATIVE ASPHALTENE FRACTIONS BY ¹H NMR**
*Lina Constanza Navarro Quintero, Samir Nasser, Peter Rudolf Seidl**, Sonia M. C. Menezes, Katia Z. Leal, Claudio Ziglio, Fábio H. S. Rodrigues and Ljubica Tasic
- Tr 47 – **NIMESULIDE ASSAY IN COMMERCIAL DRUGS USING q-NMR SPECTROSCOPY**
*Alberto de Andrade R. Mota and Claudia J. Nascimento**
- Tr 48 – **NMR METHOD FOR THE DETERMINATION OF NEVIRAPINE IN PHARMACEUTICAL FORMULATIONS**
*Érika Pereira de Aquino**, Nathalia Vêtere Melo, Erika Martins de Carvalho and Jochen Junker
- Tr 49 – **NMR ON THE MULTICOPPER OXIDASE Fet3p**
*Maria Eugenia Zaballa**, Lynn Ziegler, Daniel J. Kosman and Alejandro J. Vila
- Tr 50 – **NMR STRUCTURE ELUCIDATION AND QUANTIFICATION OF ACTIVES COMPOUNDS ISOLATED FROM THE ETHANOLIC EXTRACT OF ZEYHERIA TUBERCULOSA (VELL)**
*Antônio Euzébio G. Sant'Ana**, Maria Amélia L. dos Santos and Edson de S. Bento
- Tr 51 – **NMR STRUCTURE OF THE HUMAN PROTEIN SBDS**
*Ana-Carolina de Mattos Zeri**, Juliana Oliveira, Maurício M. Sforça, Tharin Blumenschein and Nilson Zanchin
- Tr 52 – **NMR STUDIES OF BETA-DIKETONE INTERACTIONS - THE HYDROGEN-BONDING OF THE ENOL TAUTOMERS OF SOME DIMERS OF 3-SUBSTITUTED PENTANE-2,4-DIONES**
Queli A. R. de Almeida, Joel Jones Junior, Erika M. de Carvalho and Flavia M. da Silva*

- Tr 53 – **NMR TECHNIQUES IN THE LIMONOIDS STRUCTURES DETERMINATION**
Vanessa Gisele Pasqualotto Severino, João Batista Fernandes*, Paulo Cezar Vieira and M. Fátima das G. F. da Silva
- Tr 54 – **NMR-DERIVED RESTRAINED MOLECULAR DYNAMICS USED TO STUDY BINDING OF THE ANTICOCCIDIAL PEPTIDE PW2 TO MICELLES AND LIPID BILAYER**
*Gomes-Neto F. *, Valente A. P. and Almeida, F.C.L.*
- Tr 55 – **ONLINE NMR PROCESSING PLATFORM FOR THE MANAGEMENT OF SPECTROSCOPIC INFORMATION**
*Andrés Castillo, Luc Patiny and Julien Wist**
- Tr 56 – **PARAHYDROGEN INDUCED POLARIZATION OF BARBITURIC ACID DERIVATIVES. ¹³C HYPERPOLARIZATION STUDIES**
Meike Roth, Rodolfo Acosta, Joachim Bargon, Hans W. Spiess, Achim Koch and Kerstin Münnemann*
- Tr 57 – **PRELIMINARY ASSESSMENT OF ORANGE LEAVES AFFECTED BY CITRUS CANCKER THROUGH NMR AND CHEMOMETRIC ANALYSIS**
*Lorena Mara A. e Silva, Elenilson de G. Alves Filho, Luciano Morais Lião and Glaucia Braz Alcantara**
- Tr 58 – **PREPARATION OF POLYCARBONATE/CLAY NANOCOMPOSITE FILMS AND EVALUATION BY PROTON RELAXATION TIME DISTRIBUTION**
*Pedro Paulo Merat and Maria Inês Bruno Tavares**
- Tr 59 – **PREPARATION OF POLY(ETHYLENE-CO-VINYL ACETATE) /ORGANOCLAY NANOCOMPOSITES AND CHARACTERIZATION BY NUCLEAR MAGNETIC RESONANCE OF LOW FIELD**
Rodrigo Altoé, Maria Inês Bruno Tavares and Roberto Pinto Cucinelli Neto*
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