Applications of NMR in Industry Conference

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PROGRAM GUIDE



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Conference Proceedings Link

Please use the link below to access copies of the speaker presentations that have been submitted to date, as well as conference agendas, poster abstracts, speaker information and sponsor and exhibitor websites. Following the conference, we will send out this link via email containing any updated presentations and/or late submissions.

Please note that the link will only remain active for 6 weeks after the meetings conclude.

CONFERENCE PROCEEDINGS LINK

Link: http://cii-resource.com/NMR-04-01/login.asp

User Name: Your email address

Password: nmr167300 (please note: passwords are case sensitive)

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IVIOLIGAY, I COLGALY 13	Monday	/, February	/ 15
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4:30 pm Pre-Conference Registration (Raphael Foyer)

5:30 Welcome Reception in the Exhibit Hall with Poster Viewing, Even and Odd Numbered Posters

(Raphael B)

6:45 End of Day

Tuesday, February 16

(Raphael A)

8:00 am Conference Registration and Morning Coffee (Raphael Foyer)

8:45 Chairpersons' Welcome

Gonzalo Hernandez, Vis Magnetica NMR Consulting

Kristie M. Adams, DuPont

PETROCHEMICAL/REFINERY

8:50 Chairperson's Remarks

Katherine Wu, Albemarle Corporation

9:00 Solving Problems in the Oil Industry by NMR

Sonia Menezes, Ph.D., Senior Research Consultant, Chemistry, Petrobras

9:30 Characterization of Solid Materials by DNP Enhanced Solid State NMR Spectroscopy

Marek Pruski, Ph.D., Senior Scientist; Professor, Department of Chemistry, Ames Laboratory; Iowa State

University

10:00 Earth Subsurface Exploration by Magnetic Resonance for Oilfield Applications: No Longer a Niche

Service

Nate Bachman, Ph.D., Physicist and Project Manager, Engineering, Schlumberger

10:30 Coffee Break in the Exhibit Hall with Poster Viewing, Even Numbered Posters (Raphael B)

APPLICATIONS OF NMR FOR PHARMACEUTICALS I

11:20 Chairpersons' Remarks

Joe Ray, Baxter Healthcare Corporation

Daron Freedberg, CBER, FDA

11:30 NMR Approaches in Bioconjugation: Toward Better Characterized Vaccines

Kelly Sackett, Ph.D., Senior Scientist, Biotherapeutics, Pharmaceutical Sciences, Pfizer



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Tuesday, February 16

(Raphael A)

12:00 pm NMR Profiling and Comparison of Higher Order Structure (HOS) of Protein Therapeutics

Kang Chen, Ph.D., Staff Fellow, Center for Drug Evaluation and Research, FDA

12:30 Biosimilar Structural Comparability Assessment by NMR: From Small Proteins to Monoclonal

Antibodies

Bostjan Japelj, Ph.D., Senior Scientist, Protein Biophysics and Bioinformatics, Sandoz Biopharmaceuticals

BRUKER LUNCHEON PRESENTATION

1:00 Software Assisting Your Small Molecule Workflow

Sandra Groscurth, Ph.D., Bruker BioSpin AG

Kim Colson, Ph.D., Business Development Manager, Research & Development

Division, Bruker BioSpin



1:45 Session Break

QNMR

2:30 Chairpersons' Remarks

Torsten Schoenberger, Bundeskriminalamt

John Marino, NIST

2:40 Between Metabolomics and Metrology: The Development Paths of Quantitative NMR

Guido Pauli, Pharm.D., Ph.D., Professor and University Scholar, College of Pharmacy, University of Illinois, Chicago

3:10 Recent Research Developments in the Certification of Organic Reference Materials by Quantitative

NMR at the Highest Metrological Level

Markus Obkircher, Ph.D., Senior Manager, R&D, SigmaAldrich

3:40 Polyethylene Glycol Quantitation in Biofluids Supporting Drug Discovery

Purnima Khandelwal, Ph.D., Senior Research Investigator, Discovery Analytical Sciences, Bristol-Myers Squibb

4:10 Networking Reception in the Exhibit Hall with Poster Viewing, Odd Numbered Posters (Raphael B)

5:10 End of Day



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	Wed	lnesd	ay, F	ebrua	ry 17
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(Raphael A)

8:00 am Morning Coffee (Raphael Foyer)

8:45 Chairpersons' Welcome

Gonzalo Hernandez, Vis Magnetica NMR Consulting Kristie M. Adams, DuPont

>> POSTER SPOTLIGHTS <<

8:50 Chairperson's Remarks

Jim DeFelippis, The Dow Chemical Company

9:00 35Cl Dynamic Nuclear Polarization Solid-State NMR of Active Pharmaceutical Ingredients

Robert W. Schurko, University of Windsor

9:20 Aqueous Mixture Characterization Using Selective 1D Total Correlation Spectroscopy (selTOCSY)

Nathan Rau, Dow Chemical Company

9:40 NMR Relaxometry Fingerprinting of Synthetic Materials Using a Benchtop NMR System

Philipp Moerchel, Research Center for Magnetic Resonance Bavaria (MRB)

10:00 Coffee Break in the Exhibit Hall with Poster Viewing, Even Numbered Posters (Raphael B)

SOLIDS

10:50 Chairperson's Remarks

Michael C. Davis, Bridgestone Americas Center for Research and Technology

11:00 The Use of NMR in Kidney Stone Disease Risk Assessment

Graham Jackson, Ph.D., Professor, Chemistry, University of Cape Town

11:30 Application of Advanced Solid State NMR Techniques for Structure Determination of Technical

Catalysts

Torsten Gutmann, Ph.D., Staff Scientist, Chemistry, Technical University Darmstadt

12:00 pm Solid State NMR Investigations of Silane Silica Interactions in Cured Elastomers

Michael R. Beaulieu, Ph.D., Materials Research Scientist, Bridgestone Americas Center for Research and

Technology

JEOL USA LUNCHEON PRESENTATION

12:30 Adventures with Sparse Sampling and Cool Adiabatic Experiments

Ron Crouch, NMR Applications Consultant, JEOL USA

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Solutions for Innovation

1:15 Session Break



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Wednesday, February 17

(Raphael A)

LOW-FIELD/COMPACT NMR

End of Day

7:15

2:00	Chairperson's Remarks	
	David Cistola, University of North Texas Health Science Center	
2:10	Dynamics and Wettability of Petroleum Fluids in Microporous Shale Oil Rocks: A Fast Field Cycling NMR Relaxometry Approach	
	Jean-pierre Korb, Ph.D., Director of Research, CNRS, Physics of Condensed Matter Laboratory, Ecole Polytechnique	
2:40	New Frontiers in Medical Diagnostics by T2MR®	
	Eugenio Daviso, Ph.D., Senior NMR Scientist, T2 Biosystems	
3:10	Rapid Determination of Fat Content in Microbial Biomass or Biomeal by Time Domain NMR An-Ni Chang, Ph.D., Analytics, DSM Nutritional Products	
3:40	Refreshment Break in the Exhibit Hall with Poster Viewing, Odd Numbered Posters (Raphael B)	
EXOTICA		
4:35	Chairperson's Remarks	
	John Edwards, Process NMR Associates, LLC	
4:45	Heavy Oil Viscosity Predictions from Low Field NMR Magdalena Sandor, Ph.D., Halliburton	
5:15	Spin Diffusion Editing for High Order Structure Fingerprints of Antibodies	
	Qin Zou, Ph.D., Senior Principal Scientist, Analytical Research and Development, Pfizer, Inc.	
5:45	Integrated Perfusion Systems for In Situ NMR Metabolomics of Microfluidic Cell Cultures Ali Yilmaz, Ph.D., Research Fellow, Chemistry, University of Southampton	
6:15	Networking Reception in the Exhibit Hall with Poster Viewing, Even Numbered Posters & Last Chance to Drop Off Your Entry for the Spectrum Contest (Raphael B)	



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Thursday, February 18

(Raphael A)

8:15 am Morning Coffee (Raphael Foyer)

8:45 Chairpersons' Welcome

Gonzalo Hernandez, Vis Magnetica NMR Consulting

Kristie M. Adams, DuPont

FOOD APPLICATIONS

Adriana Carvalho de Souza, DSM Biotechnology Center

9:00 Use of NMR as an Advanced Analytical Tool to Interpret Processing-Induced Changes during

Manufacture of Milk Products and Dairy Ingredients

Mattia Boiani, Walsh Fellow, Chemistry and Technology, Teagasc

9:30 Rapid Quantitative NMR Analysis of Oils to Combat Edible Oil Adulteration

Sue Wang, Ph.D., Manager, BDL, ITRI

10:00 Shear-Induced Flow Behavior of Food Dispersions as Viewed by Rheo-MRI

John Van Duynhoven, Ph.D., Head, Spectroscopy & Imaging Group, Unilever

10:30 Coffee Break in the Exhibit Hall with Poster Viewing, Odd Numbered Posters (Raphael B)

PLANT PRODUCTION PROBLEM SOLVING

11:20 Poster Awards Announced and Spectrum Contest Answer Revealed with Prizes Awarded

Poster awards provided by MRC / Wiley

11:25 Chairpersons' Remarks

Jim DeFelippis, The Dow Chemical Company

Molly Bohlen, Procter & Gamble

11:30 Online NMR Spectroscopy as a Reference Tool for Model Developments – Successful Approaches in

Process Analytical Technology

Klas Meyer, Research Assistant, Division 1.4 Process Analytical Technology, BAM Federal Institute for Materials Research and Testing

12:00 Utilizing 1D Correlation (NOE/TOCSY) and Database Techniques for Fast Structure Elucidation and

Quantitation in a Production Environment

James Surface, Ph.D., NMR Team Leader, Analytical, PPG Industries



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Thursday, February 18

(Raphael A)

ASPECT IMAGING LUNCHEON PRESENTATION

12:30 Online Process NMR Applications

Tal Cohen, Director, NMR Division, Aspect Imaging



1:15 Session Break

APPLICATIONS OF NMR FOR PHARMACEUTICALS II

2:00 Chairpersons' Remarks

Kathleen Farley, Pfizer, Inc. Daron Freedberg, CBER, FDA

2:10 Practical NMR Applications for Structure Assessment of Monoclonal Antibody Therapeutics

Robert Brinson, Ph.D., Research Chemist, Institute for Bioscience and Biotechnology Research (IBBR), NIST

2:40 Residual Dipolar Couplings to Assist Structural Analysis in Drug Discovery

Roberto Gil, Ph.D., Research Professor & Director, NMR Facility, Chemistry, Carnegie Mellon University

3:10 The Changing Role of NMR in Drug Discovery: A View from the Perspective of a Drug Metabolism

Scientist

Greg Walker, Senior Principal Scientist, PDM, Pfizer

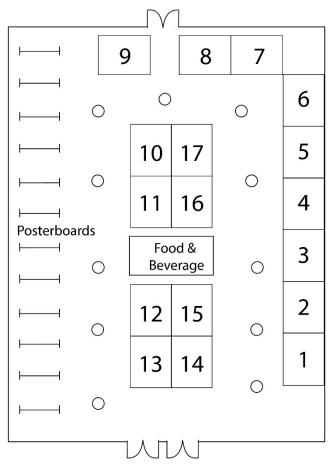
3:40 End of PANIC 2016



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Floor Plan, Exhibit and Poster Schedule

[Location: Raphael B]



COMPANY BOOTH	
Advanced Chemistry Development (ACD/Labs)10	
Anasazi Instruments Inc. 1	
Bruker Corporation	
Chenomx Inc5	
COSA Xentaur Corporation9	
HTS-1104	
JEOL USA, Inc. 11	
Magritek	
Mestrelab Research, S.L15	
MilliporeSigma6	
Nanalysis Corporation8	
Oxford Instruments2	
Quantum Design14	
Stelar	
Wilmad Labglass3	

ENTRANCE

KEY

- 8 x 10 Exhibitor Booth
- → Poster Boards
- O Cocktail Table

Exhibit and Poster Hours		
Monday		
5:30 – 6:45 pm	Welcome Reception - <i>Even <u>and</u> Odd Posters</i>	
Tuesday 10:30 – 11:20 am	Coffee Break - <i>Even Posters</i>	
4:10 – 5:10 pm	Networking Reception - <i>Odd Posters</i>	
Wednesday		
10:00 - 10:50 am	Coffee Break - <i>Even Posters</i>	
3:40 – 4:35 pm	Refreshment Break - <i>Odd Posters</i>	
6:15 - 7:15 pm	Networking Reception - Even Posters & Last Change to Drop Off Your Entry for the Spectrum Contest	
Thursday	0.50	
10:30 – 11:20 am	Coffee Break - Odd Posters	

Exhibit hours are subject to change.



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Sponsor & Exhibitor Company Descriptions

Advanced Chemistry Development, Inc. (ACD/Labs)

Booth 10

8 King Street East, Suite 107 Toronto, ON M5C 1B5 Canada 416.368.3435

www.acdlabs.com

Advanced Chemistry Development, Inc., (ACD/Labs) is an informatics company that provides solutions in support of R&D. Our software platforms unify analytical and chemical information in a collaborative environment; and provide tools that enable scientists to extract, capture, and apply knowledge from analytical experiments and predicted molecular property data.

Anasazi Instruments Booth 1

4101 Cashard Avenue, #103 Indianapolis, IN 46203 317.783.4126

Manufactures highest resolution, sensitivity and stability permanent magnet based NMR instruments. The Eft-60/90MHz models can be tailored to users' needs, such as ultra-high sensitivity 1H, two channel 1H/13C or 1H/31P and two channel multinuclear 1H/19F/X (tunable X). Both instruments are available with a robotic sample changer for unattended

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Bruker BioSpin Booth 12 & 13

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Bruker offers the world's most comprehensive range of NMR research tools. With over 50 years of experience, Bruker remains strongly committed to meeting its customers' needs by continuing to revolutionize the design, manufacture and distribution of life science, process control and analytical research tools based on magnetic resonance core technology.

Cambridge Isotope Laboratories, Inc.

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Chenomx Inc. Booth 5

10230 Jasper Avenue, Suite 4350 Edmonton, AB T5J 4P6 Canada 780.432.0033

www.chenomx.com

Chenomx supports quantitative metabolite measurements with NMR. Chenomx patented Targeted Profiling turns complex MR spectra into tables of metabolites and their concentrations. The quantitative approach to metabolomics facilitates the discovery and testing of marker patterns for diagnostics, cell metabolism and qNMR applications. Chenomx offers both software licensing and analysis services.

COSA Xentaur Corporation

Booth 9

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HTS-110 Limited Booth 4

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JEOL USA, INC Booth 11

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J S Research, Inc.

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Magritek Booth 16

6440 Lusk Boulevard, Suite 108 San Diego, CA 92121 855.667.6835

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Magritek is a world leading company developing and manufacturing portable NMR solutions for education, research and industrial applications. SpinsolveTM is the first benchtop NMR instrument capable of multinuclear (1H, 19F, 31P, 13C) and multidimensional NMR that does not require cryogenics and is maintenance free. Magritek is exhibiting Spinsolve®, a revolutionary benchtop NMR spectrometer that provides exceptional performance in a low-cost, convenient and compact package.

Mestrelab Research Booth 15

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mestrelab.com

Mestrelab Research specializes in the development of software for the processing, analysis and databasing of Analytical Chemistry data.

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Booth 6

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Oxford Instruments Booth 2

300 Baker Avenue, Suite 150 Concord, MA 01742 978.369.9933

www.oxford-instruments.com

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Stelar Booth 17

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Booth 3

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Poster Presenters

(Location: Raphael B)

Presenting Monday, February 15th through Thursday, February 18th

Advanced Chemistry Development, Inc.

Sergey Golotvin; Rostislav Pol; Brent Pautler; Joe DiMartino; Arvin Moser; and <u>Patrick Wheeler</u>: *Novel Means for Identification and Quantitation of Mixture Components by NMR*

Alkermes, Inc.

2 Mark D. Trone and <u>David Wang</u>: *Drug Substance Potency Determination by Quantitative NMR (qNMR) and Low Level Impurity Quantitation with 13C–1H NMR Satellite Signals*

Amgen, Inc.

3 Krishnakumar Ranganathan; Yuan-Qing Fang; Richard D. Crockett; Stephen A. Osgood; Sheng Cui; and <u>Tsang-Lin Hwang</u>: Studies of Coupling Kinetics and Conversion Rates and Correlations to Color Tests for Solid Phase Peptide Synthesis by NMR

BAM Federal Institute for Materials Research and Testing

- 4 Patrick Gräßer; Simon Kern; Nicolai Zientek; Andrea Paul; Michael Maiwald; and <u>Klas Meyer</u>: Field Integration of Benchtop NMR Instruments for Online Monitoring and Process Control of a Modular Industrial Reaction Step
- 5 Simon Kern; Michael Maiwald; and <u>Klas Meyer</u>: *CONSENS Integrated Control and Sensing for Sustainable Operation of Flexible Intensified Processes*
- 6 Klaus Rademann; Michael Maiwald; and <u>Klas Meyer</u>: *qNMR Under Pressure Applications on Liquefied Gases and Mixtures*

Bristol-Myers Squibb

Adele Patterson; Yande Huang; Scott A. Miller; and <u>Qingmei Ye</u>: Structural Characterization and Two-Dimensional HSQC NMR Quantitative Determination of the Degradation Product of PVP/VA Copolymer

Bruker BioSpin

- 8 Brian Killday and <u>Kimberly L. Colson</u>: *Cell Culture Media: NMR Approaches to Evaluating Quality and Nutrient Consumption*
- 9 Till Kühn; Sebastian Wolf; Sven Brehmer; Jens Fuchser; Meike Hamester; and <u>Sandra Groscurth</u>: *Automated Structure Verification by Combining High Resolution Accurate MS with NMR Data Analysis*

Dow Chemical Company

10 <u>Nathan Rau</u>: Aqueous Mixture Characterization Using Selective 1D Total Correlation Spectroscopy (selTOCSY)

Dublin City University

11 Michael D. Mantle; Aylvin Dias; Dermot Brougham; Victor M. Litvinov; and <u>Bing Wu</u>: *Effect of H-Bonding on the Diffusion of Drug Analogue Inside Crosslinked Hydrogel*

Duke University

Anthony A. Ribeiro; Timothy D. Spitzer; and <u>Andrea M. Sefler</u>: A Practical Survey of the Indirect 1-Bond H-C Correlation Experiments Available Within VnmrJ 4.2/Chempack 7.1



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Genentech, Inc.

13 Matt Delsman; Nick Magarian; Yung-Hsiang Kao; and <u>Ken Skidmore</u>: *Nanogram/mL Analysis of Formulated Protein Drug Product: Combating Lyophilizer Leaks Using NMR*

INNIT SAS

Laetitia Le Falher; Delphine Lioger; Hervé This; and <u>Camille Doyen</u>: *Thermal Degradation of Saccharides in Water Analyzed by In Situ 1H Quantitative NMR*

ISOThrive, LLC

15 <u>Lee Madsen II</u>: Evaluation of a Turn-Key Variable Temperature (VT) Probe for Low-Field Applications

JEOL RESONANCE, Inc.

Naoki Saito; Taichi Yamazaki; Hiroaki Sasakawa; Takeshi Saito; and <u>Takako Suematsu</u>: *The Influence of Data Processing on Results of qNMR Interlaboratory Comparison Study*

Korea Basic Science Institute

17 Hyun Na Kim and Oc Hee Han: Interaction of Side-Chains with Water in Swollen Nafion Polymer Electrolyte Membranes

Magritek, Inc.

- F. Casanova; A. Coy; B. Manz; S. L. Moore; J. Perlo; and <u>Paul Bowyer</u>: *Diffusion-Ordered Benchtop NMR Spectroscopy*
- E. McCarney; A. Coy; F. Casanova; B. Manz; S. L. Moore; and <u>Paul Bowyer</u>: *Application of Benchtop NMR Spectroscopy to the Identification and Quantitation of Nutraceuticals and Pharmaceuticals*

Mestrelab Research S.L.

- Torsten Schoenberger and Michael A. Bernstein: Automation of qNMR Analysis for Dissimilar Sample Mixtures
- Anna Gerdova; David Williamson; and <u>Michael A. Bernstein</u>: *Development of an Automated Biodiesel Analysis Tool Using Data Acquired Using Low-Field NMR Spectrometers*

Nanalysis Corporation

Michael A. Bernstein; Andrew R. Hillson; and <u>Susanne D. Riegel</u>: *Automated Analysis:Integration of Benchtop NMR with Automated Processing and Quantification*

National Institute of Advanced Industrial Science and Technology (AIST)

Takeshi Saito; John Warren; Stephen Davies; Masahiko Numata; and <u>Taichi Yamazaki</u>: *An Inter-Comparison Study of Data Acquisition and Processing in qNMR Measurement Among National Metrology Institutes*

National Institute of Chemistry

- 24 Janez Plavec and Gregor Ilc: Structural Insights into Signal Switch of TROP 2
- Kristina N. Farrugia; Maria Cardona; David C. Magri; Janez Plavec; and <u>Damjan Makuc</u>: *NMR Spectroscopic Studies* of (De)protonation Mechanisms in Azobenzene and Thiosemicarbazide Based Anion Chemosensors

National Institute of Standards and Technology

Michael A. Boss; Kathryn E. Keenan; Stephen E. Russek; and <u>Karl F. Stupic</u>: *Developing Quantitative T1 Measurements for Traceable Relaxometery in NMR and MRI*



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Northeastern University

27 Sergiy Tyukhtenko; Alexandros Makriyannis; and <u>Jason J. Guo</u>: *Hydrogen Bonded Histidines as Sensitive Probes for Protein-Based NMR Drug Discovery*

Pfizer, Inc.

Qin Zou and Robert Kutlik: 1D 1H NMR Spectroscopy Method for Monoclonal Antibody Higher Order Structure Fingerprinting

Princeton University

D. Ferlisi; K. Conover; M. Mohr; P. K. Sirois; V. A. Massi; I. Pelczer; S. Ralston; and Minhaz Mahbub: Time-Domain NMR Analysis of Composition of Grass and Hay

Research Center for Magnetic Resonance Bavaria (MRB)

Markus Hildenbrand; Karl-Heinz Hiller; Peter Jakob; and <u>Philipp Moerchel</u>: *NMR Relaxometry Fingerprinting of Synthetic Materials Using a Benchtop NMR System*

Stelar Srl

- M. Pasin; R. Steele; A. Marchi Netto; M. Farah; E. A. Rössler; and <u>Gianni Ferrante</u>: Fast Field Cycling NMR Relaxometry Applied to Understand the Dynamics of Industrial Branched Polypropylene Polymers
- G. Ferrante; D. Lurie; L. Broche; J. Ross; P. Vanezis; R. Wortley; R. Morgan; R. Steele; and <u>Saravanan Kanniappan</u>: Using Fast Field Cycling (FFC) NMR Relaxometry and FFC-MRI for the Determination of Post-Mortem Interval: Preliminary Study Measuring Post-Mortem Decomposition Rates
- Nopparat Vorapalawut; Benjamin Nicot; M. Pasin; R. Steele; G. Ferrante; and <u>Jean-Pierre Korb</u>: *Applications of Fast Field Cycling NMR Relaxometry in the Petroleum Industry*

U.S. Army, Edgewood Chemical Biological Center

34 William R. Creasy and <u>David J. McGarvey</u>: Quantitative C-13 NMR Analysis of Sulfur Mustard Materials

Universidad Autónoma de Madrid

35 <u>Ernesto Brunet</u>: Benchtop NMR: A Technologically-Tweaked, Incredible Going-Back to NMR Origins

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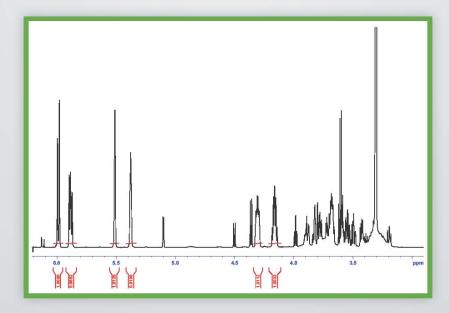
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