

PROGRAMME

Sunday, September 10:

18.00-22.00 **Registration** (Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, Warszawa)

Monday, September 11:

10.15-10.30 **Opening Ceremony:**

Krystyna Kamieńska-Trela – Chairperson of the Organizing Committee (*Institute of Organic Chemistry, Polish Academy of Sciences, Warszawa*)

Marek Chmielewski – Director of the Institute of Organic Chemistry Polish Academy of Sciences

SESSION I: Chairman – Marek Chmielewski (*Institute of Organic Chemistry, Polish Academy of Sciences, Warszawa*)

10.30-11.15 **Philip W. Kuchel, David Szekely, Christoph Naumann, Bogdan E. Chapman, and William A. Bubb**
School of Molecular & Microbial Biosciences, University of Sydney, Australia

[FL-1] NMR Residual Quadrupolar Splittings of Cations and H-Bond Induced Shifts in Red Blood Cells: Studies of Ionic Mobility and Rapid Membrane Transport

11.15-12.00 **Edvards Liepinsh**
Latvian Institute of Organic Synthesis, Department of Physical-Organic Chemistry, Latvia

[FL-2] Some New Protein Structures Determined by NMR

12.00-12.30 **Coffee break**

SESSION II: Chairman – Jan Schraml

12.30-13.15 **Janez Plavec**
NMR Centre, National Institute of Chemistry, Slovenia

[FL-3] Insights into Localization and Cation Mobility within Dimeric G-Quadruplexes by NMR

13.15-13.35

Lucjan Sobczyk, A.F. Pozharskii , V.A. Ozeryanskii, A. Filarowski

Faculty of Chemistry, University of Wrocław, Poland

[L-4]

Factors Affecting the Bridge Proton NMR Chemical Shift in Protonated Naphthalene Proton Sponges

13.35-13.55

Patrick Groves, Agnieszka-Strzelecka-Kiliszek, Angeles Canales, Katalin E. Kövér, Gyula Batta, F. Javier Cañada, Joanna Bendorowicz-Pikuła, Jesús Jiménez-Barbero, Sławomir Pikuła

Centro de Investigaciones Biológicas, CSIC, Dept. of Structure and Function of Proteins, Madrid, Spain

[L-5]

Analysis of Annexin-Nucleotide Complexes by NMR

14.00-15.00

Lunch

SESSION III: Chairman – Karol Jackowski

15.00-15.45

Helena Dodziuk, M. Ostrowski, J. Jaźwiński, P. Kuś

Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland

[FL-6]

Unusual Structure and NMR Spectra of Cyclophanes with Short Bridges

15.45-16.30

Wiktor Koźmiński, Krzysztof Kazimierczuk, Anna Zawadzka, Igor Zhukov

Department of Chemistry, Warsaw University, Warsaw, Poland

[FL-7]

Fast Multidimensional NMR – Multidimensional Fourier Transform of Arbitrarily Sampled NMR Data Sets

16.30-17.15

Thomas Zellhofer

Varian Deutschland GmbH, Darmstadt, Germany

[FL-8]

(a title will be submitted later)

18.00-21.00

Conference mixer

Tuesday, September 12:

SESSION IV: Chairman – Philip W. Kuchel

9.00-9.45 **Stephan Grzesiek, M. Allan, F. Cordier, S. Dames, D. Häussinger,
P. Jensen, J. Kahmann, H.J. Sass, and N. Vajpai**

Biozentrum, University of Basel, Basel, Switzerland

[FL-9] NMR as a Quantitative Tool to Study Interactions in Biomacromolecules

9.45-10.30 **Marek J. Potrzebowski**

*Centre of Molecular and Macromolecular Studies, Polish Academy of
Sciences, Łódź Poland*

[FL-10] NMR Study of Structure and Dynamics of Amino Acids and Small Peptides
in the Solid State

10.30-11.15 **Stefan Jurga**

Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

[FL-11] NMR in Soft Matter

11.15-11.40 ***Coffee break***

SESSION V: Chairman – Marek Potrzebowski

11.40-12.25 **Joseph Kowalewski**

Arrhenius Laboratory, Stockholm University, Stockholm, Sweden

[FL-12] Small Molecules and Carbon-13 Relaxation outside of Extreme Narrowing

12.25-13.10 **Karol Jackowski, Włodzimierz Makulski and Marcin Wilczek**

University of Warsaw, Department of Chemistry, Warszawa, Poland

[FL-13] ^{17}O and ^1H Magnetic Shielding and Spin-Spin Coupling
of ^{17}O -Enriched Water in the Gas Phase

13.10-13.30 **Danuta Kruk**

*Institut für Festkörperphysik, TU Darmstadt, Darmstadt, Germany and
Institute of Physics, Jagiellonian University, Krakow, Poland*

[L-14] Field Dependent Nuclear Spin Relaxation as a Tool for Investigating
Dynamics of Complex Spin Systems

13.30-14.00 **Marta Bugaj, Krystyna Kamińska-Trela**

Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland

[L-15]	Low Temperature Measurements of Carbon-Carbon Spin-Spin Couplings in <i>S-cis</i> and <i>S-trans</i> Rotamers of Enaminoketones; Comparison with DFT Computations
14.00-15.00	Lunch
SESSION VI:	Chairman – Joseph Kowalewski
15.00-15.45	<u>Lech Kozerski</u>, Wojciech Bocian, Elżbieta Bednarek, Jerzy Sitkowski, Anna Bzowska, Robert Kawęcki <i>Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland</i>
[FL-16]	NMR Investigations of Human Insulin Aggregation and Structure
15.45-16.30	<u>Manfred Spraul</u> and Hartmut Schäfer <i>Bruker BioSpin, Germany</i>
[FL-17]	The Use of NMR in Metabonomics
16.30-16.50	<u>Lidia Latanowicz</u>, Zofia Gdaniec <i>Institute of Biotechnology and Environmental Sciences, University of Zielona Góra, Zielona Góra, Poland</i>
[L-18]	Internal and Overall Molecular Motions in Solution Studied by Carbon-13 Spin-Lattice Relaxation and Proton-Proton Cross-Relaxation Rates
16.50-17.10	<u>Rafał Kuźmich</u>, Wacław Kołodziejwski <i>Medical University of Warsaw, Faculty of Pharmacy, Warszawa, Poland</i>
[L-19]	¹³ C CP MAS NMR Characterization of C-Methylcalix[4]resorcinarene/Acetonitrile Solvate
17.10-17.30	<u>Jarosław Gajda</u>, Marek J. Potrzebowski, Włodzimierz Ciesielski <i>Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Łódź Poland</i>
[L-20]	³¹ P Solid State NMR Study of Bioorganic Phosphates
17.30-18.00	Coffee break
18.00-20.00	Poster session

Wednesday, September 13:

SESSION VII: Chairman – Stephan Grzesiek

9.00-9.45 Jan Schraml

Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic, Prague, Czech Republic

[FL-21] Two Current Topics in ^{29}Si - NMR of Liquids

9.45-10.30 Andrzej Ejchart

Institute of Biochemistry and Biophysics, Polish Academy of Sciences, Warsaw, Poland

[FL-22] Application of Nuclear Magnetic Relaxation to the Backbone Dynamics of S100A1 Protein

10.30-10.50 Leszek Pazderski, Jaromir Toušek, Jerzy Sitkowski, Lech Kozerski, Edward Szlyk

Nicholas Copernicus University, Faculty of Chemistry, Toruń, Poland

[L-23] ^1H , ^{13}C and ^{15}N NMR Spectra of the Cationic and Anionic Forms of 6-Mercaptopurines and the Products of Their Oxidation

10.50-11.10 Wojciech Medycki, Krystyna Holderna-Natkaniec

Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

[L-24] Rotational Tunneling in Mesitilene

11.10-11.40 Coffee break

SESSION VIII: Chairman: Wacław Kołodziejwski

11.40-12.10 Jarosław Jaźwiński

Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland

[FL-25] Chiral Adducts of Amines with Rhodium(II) Tetracarboxylates: Application of ^1H , ^{13}C and ^{15}N NMR Spectroscopy

12.10-12.30 Mariusz A. Tuz, Małgorzata Kuliszkievicz-Janus, Stanisław Baczyński, Marek Kielbiński, Bożena Jaźwiec, Iwona Prajs, Helena Śladowska

Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

[L-26] ^{31}P *in Vitro* Assay of Phospholipids of Red Blood Cells (RBC) of Patients with Hematological Cancers – Preliminary Results

- 12.30-12.50** **Rafal Latajka, Michal Jewginski, Maciej Makowski, Pawel Kafarski**
Faculty of Chemistry, Wroclaw University of Technology, Wyspianskiego
Wroclaw, Poland
- [L-27]** Spectroscopic and Theoretical Investigations of Peptides Containing Two
Dehydroamino Acid
- 12.50-13.10** ***Closing remarks***
Krystyna Kamieńska-Trela – Chairperson of the Organizing
Committee (*Institute of Organic Chemistry, Polish Academy of Sciences,*
Warszawa)
Marek Chmielewski – Director of the Institute of Organic Chemistry
Polish Academy of Sciences
- 13.10-14.00** ***Lunch***

FL- full lecture, **L-** lecture