

CENTRAL EUROPEAN NMR DISCUSSION GROUPS

17th NMR Valtice

8.-10.4.2002

Valtice, Czech Republic

PROGRAMME

Monday April 8, 2002

Afternoon 2 p.m.

- 14:00 Opening of the Conference
- 14:10 Markéta Munzarová, Vladimír Sklenář:
Parameterization of the Karplus Equation for the Glycosidic Torsion in Nucleic Acids: *Ab initio* Study.
- 14:25 Lukáš Trantírek, Erik Caha, Michael Akke, Radovan Fiala:
Base and Sugar Dynamics in GCAA RNA Hairpin Tetraloop.
- 14:40 Petr Padrta:
Refinement of d(GCGAAGC) Hairpin Structure Using One- and Two-Bonds Residual Dipolar Couplings.
- 14:55 Petr Padrta, Josef Chmelík:
Evaluation of Protein Torsion Angles Using Program MULDER.
- 15:10 Monika Nálezková, Josef Chmelík, Lukáš Žídek:
Structural Studies of Major Urinary Protein I
- 15:25 Karin Hohenthanner, Guido Pintacuda, Norbert Müller:
Progress in Application of Cross Correlated Curie Spin Relaxation for Structure Determination in Paramagnetic Proteins.

15:40 Break

- 16:15 Richard Hrabal, Václav Veverka, Jan Lang, Helena Bauerová, Iva Pichová:
Progress in Structural Study of Protease from Mason-Pfizer Monkey Virus.
- 16:30 Václav Veverka, Jan Lipov, Michaela Rumlová, Tomáš Ruml, Richard Hrabal:
NMR Study of Phenotypically Relevant Mutants of Matrix Protein from Mason-Pfizer Monkey Virus.
- 16:45 Dana Kurková, Jaroslav Kříž, Pavel Schmidt, Jiří Dybal, José Carlos Rodríguez-Cabello, Matilde Alonso:
Inverse temperature transition in poly(Gly-Val-Gly-Val-Pro) and poly(Ala-Val-

Gly-Val-Pro) studied by NMR spectroscopy.

17:00 Jiří Brus, Jiří Dybal:
 ^1H - ^1H Interatomic Distance Measured by Multidimensional CRAMPS Experiments.

17:15 Gábor Szalontai:
Residual Dipolar Couplings in ^{31}P and ^{29}Si MAS Spectra of Co(I) Complexes.

18:00 Dinner

20:00 Get-together party in wine cellar sponsored by Varian

Tuesday April 9, 2002

Morning 8.30 a.m.

8:30 Jiří Vlach, Veronika Michlová, Jan Lang:
Determination of Calix[4]arene Complex Geometry Using Full Relaxation Matrix.

8:45 Hana Dvořáková, Jan Lang, Pavel Lhoták:
NMR Study of Conformational and Dynamic Properties of Thiacalix[4]arenes: the Pinched Cone/Pinched Cone Conversion.

9:00 Tamás Gáti, Gábor Tóth, Helmut Duddeck, Shahid Malik:
Complexation of Selenium to (R)-Rh₂(MTPA)₄: Thermodynamics and Stoichiometry by ^1H , ^{13}C and ^{77}Se NMR.

9:15 József Kovács, Gábor Tóth, András Simon, Albert Lévai, Erich Kleinpeter:
Stereochemistry of 3-Arylidene-1-thioflavan-4-on sulfoxides and sulfones by ^1H , ^{13}C , ^{17}O NMR and Quantum-Chemical Calculations.

9:30 Antonín Lyčka, Jaroslav Holeček:
 ^{17}O NMR Spectra of Some Organotin(IV) Acetates.

9:45 Tomáš Lébl, Jaroslav Holeček
The Investigation of Intramolecular Donor-Acceptor Interaction in 3-Methoxypropylstannanes by Means of Long-Range $^n\text{J}(^1\text{H}-^{119}\text{Sn})$ Coupling Constants.

10:00 Break

- 10:30 Ján Imrich, Karel D. Klika, Nad'a Prónayová, Juraj Alföldi, Tibor Liptaj, Juraj Bernát, Pavol Kristian, Kalevi Pihlaja, Mária Vilková, Eva Balentová:
NMR Properties of New Spirocyclic and Heterocyclic Acridine Derivatives.
- 10:45 Radek Marek, Marcela Lukášková, Jaromír Toušek, Jiří Brus, Zdeněk Trávníček:
Protonation and Tautomerism of 6-Benzylaminopurine Derivatives.
- 11:00 Franc Perdih, Alojz Demšar, Janez Košmrlj, Andrej Pevec:
NMR Studies of the Solvation of Lithium Cation in $[\{\text{Li}(\text{Cp}^*_2\text{Ti}_2\text{F}_7)(\text{L})\}_2]$.
- 11:15 Miroslav Holík, Miloslav Nechvátal:
Computations with Three-dimensional Matrix of Chemical Shift Data.

12:00 Lunch

14:00 Excursion to the 'Cross' wine cellar

16:30 Information about new products of our sponsors

18:30 Dinner

20:00 Meeting of the NMR Discussion Groups - refreshment sponsored by Bruker and Scientific Instruments Brno

Wednesday April 10, 2002

Morning 8.30 a.m.

- 8:30 V. Mlynárik, Z. Starčuk, Z. Starčuk, Jr., S. Gruber, E. Moser:
Proton NMR Spectroscopy of Human Brain at 3 Tesla.
- 8:45 Zoltán Berente, Erzsébet Ósz, Balázs Sümegi:
In vivo and *in situ* Metabolic Studies Using Magnetic Resonance Spectroscopy (MRS) and Imaging (MRI).
- 9:00 Milan Mazur:
„Lens Effect“ in Magnetic Resonance Spectroscopy.
- 9:15 Lothar Brecker, Ulrich Zähringer:
High Resolution NMR Analysis of Lipid A – A Methodological Approach Towards the NMR Analysis of a Charged Amphiphile.

- 9:30 Christian Steindl, Christina Schäffer, Paul Messner, Norbert Müller:
NMR – Structure Elucidation of the Carbohydrate Part of a Secondary Cell Wall
Polymer (SCWP).
- 9:45 Vilko Smrečki, Norbert Müller :
An *ab initio* Study of N-15 CSA Tensors in Peptides.
- 10:00 Gy. Batta, F. Sztaricskai, S.S. Printsevskaya, M.N. Preobrazehnskaya:
Cell-Wall Analogue Induced Effects in Glycopeptides.
- 10:15 M. Kuzma, P. Sedmera, V. Havlíček, A. Jegorov:
Some New Cyclic Peptides and Depsipeptides.
- 10:30 Jiřina Bohdálková, Ervín Kozubek, Miroslav Kaloč:
NMR Spectroscopy of Bituminous Coal Tars.
- 10:45 Martin Albert, Petra Feiertag, Gertraud Hayn, Helmut Hönig and Robert Saf:
Polyguanidine Biocides: A Comparative ¹H-, ¹³C- And ¹⁵N-NMR Study
Complemented by MALDI-TPF-MS Spectra.

11:00 Closing of the Conference