

## 14<sup>th</sup> NMR VALTICE - PROGRAMME

Monday	April 12, 1999	Afternoon	2 p.m.
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- 14.00 Opening of the Conference.
- 14.10 J.Lang, H.Dvoráková, I.Bartošová, P.Lhoták, I.Stibor, R.Hrabal,  
Quantitative Determination of Thiacalix[4]arene Scaffold Flexibility.
- 14.25 H.Dvoráková, J.Lang, I.Bartošová, P.Lhoták, I.Stibor, R.Hrabal,  
Conformational Behaviour of Novel Tetraalkylated Thiacalix[4]arenes.
- 14.40 J.Moravcová, R.Bláhová, H.Dvoráková, M.Tkadlecová,  
DNMR Study of a Pentafuranose with the Annelated Pyrazolidine Ring.
- 14.55 J.Havlíček, M.Hamerníková, K.Kefurt,  
NMR Investigation of Structure and Conformation of Aminodeoxyhexonolactams.
- 15.10 V.Macháček, A.Lycka, P.Šimunek, T.Weidlich,  
<sup>15</sup>N, <sup>13</sup>C and <sup>1</sup>H NMR Study of Diazonium Salts Coupling Products with Enaminones.
- 15.25 A.Ruzicka, R.Jambor, J.Holecek, A.Lycka, K.Jacob,  
Multinuclear NMR Study of Intramolecular Metal-Nitrogen Interactions in Some C,N-  
Chelate Compounds.
- 15.40 P.Šimunek, V.Macháček, A.Lycka, T.Weidlich,  
NMR Study of Structure of Products from Azocoupling Reactions of Arenediazonium  
Salts to Enamine with Tertiary Amino Group.
- 15.55 T.Weidlich,  
Substituted 2-Nitrosobenzonitriles as the Intermediates in Reaction of Nitroaromates  
with Cyanide and Methyl Cyanoacetate.
- 16.10 Break
- 16.40 H.Duddeck, C.Meyer, S.Rockitt,  
Chiral Dirhodium Complexes - New Auxiliaries for Chiral Recognition of Olefines,  
Nitriles and other Functionalities by NMR Spectroscopy.

- 16.55 B.Balázs, G.Tóth, P.Scheiber, P.Nemes,  
Solvent Dependent Conformations of Some Saturated Diazatricyclic Compounds and their Salts.
- 17.10 J.Kovács, A.Simon, T.Gáti, H.Duddeck, G.Tóth,  
NMR Investigation of 5 $\alpha$ - and 5 $\beta$ -Cardenolides Isolated from *Calotropis procera* and *Acokanthera spectabilis*.
- 17.25 D.Šaman, I.G.Stará, I.Starý, A.Kollárovic, F.Teplý, M.Tichý,  
NMR of Helicenes and Their Precursors.
- 17.40 M. Tichý, M.Budesínský, J.Günterová, J.Závada, J.Podlaha, I.Císarová,  
Synthesis and Stereochemistry of 5,7-Dicyano-6,7-dihydro-5H-dibenz[c,e]azepines.
- 17.55 R.Marek, D.Hocková, J.Slavík, R.Dommissé, V.Sklenár,  
<sup>15</sup>N NMR Study of Natural and Synthetic Nitrogen Heterocycles.
- 18.10 I.Tišlerová, J.Sejbal, Š.Vyskocil, P.Kocovský,  
An NMR Study of a Unique P,C $\Sigma$ -Coordination of 2-Dimethylamino-2'-diphenylphosphino-1,1'-binaphthyl (MAP) to Palladium.
- 18.25 V.Proks, M.Holík,  
Substituent Dependence of the Benzylideneaniline Conformation.

19.00 Dinner

20.00 Get-together party in wine cellar sponsored by Varian.

Tuesday	April 13, 1999	Morning	8 a.m.
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- 8.00 M.Mazúr,  
Quantity in Magnetic Resonance Spectroscopy - Part 2.
- 8.15 H.Hönig,  
On the Performance of Some <sup>13</sup>C-NMR-Shift-Prediction Programs with Common and Less Common Classes of Compounds.
- 8.30 N.Müller, M.Emsenhuber,

Novel Experimental Approach for the Selective Observation of Chemical Exchange.

- 8.45 J.Schraml, D.Šaman, J.Pelnár,  
VNMR\_NET
- 9.00 Á.Demeter, C.Szántay, Jr.,  
Analysis of the On-Resonance NMR Saturation Transfer Experiment in the Presence of Two-Site Exchange: The Effect of Varying RF Field Strength on Saturation Transfer Dynamic.
- 9.15 V.Mlynárik,  
NMR-Accessible Parameters of Water in Normal and Pathologic Articular Cartilage.
- 9.30 T.N.Pham, T.Liptaj, V.Mlynárik, S.Kašparová,  
*In-vivo* Determination of the Kinetic Parameters of the Creatine Kinase Reaction.
- 9.45 S.Kašpárková, T.Liptaj, Z.Braunová, V.Mlynárik, J.Kucharská, A.Gvozdjaková,  
A Study of the Creatine Kinase Reaction in Rat Brain After Prolonged Ethanol Consumption
- 10.00 Z.Starcuk, J.Horký, Z.Starcuk, Jr.  
Some Aspects of *in-vivo* <sup>1</sup>H NMR Spectroscopy.
- 10.15 Break
- 10.45 P.Sedmera, J.Volc, S.Pospíšil, L.Weignerová, V.Kren,  
NMR of Mono- and Oligosaccharides.
- 11.00 A.Demšar, S.Petricek, J.Košmrlj,  
Carboxylate Shift Tautomerisation in Zinc Complex and its Relevance to Metalloenzymes.
- 11.15 M.Emsenhuber, N.Müller,  
Influence of Cyclodextrins on the Kinetics of Tyrosyl-proline Peptide Bond cis/trans-Isomerization.
- 11.30 K.Fehér, L.Szilágyi,  
Assignments and Conformational Studies of Oligomycin Antibiotics by <sup>1</sup>H and <sup>13</sup>C

NMR.

- 11.45 M.D.Mihovilovic, G.Hattinger, J.Röhring, Ch. Hametner, P.Stanetty,  
NMR Studies of Halogenated Heteroaromatic Cross Coupling Products.
- 12.00 A.Petric,  
Unusual Products of a Nucleophilic Substitution Reaction Identified by NMR.
- 12.15 C.Szántay Jr., G.Tárkányi,  
NMR Study of the Conformational Behaviour of Vinblastine and Related Alkaloids.
- 12.30 M.Morvai, B.Podányi,  
New Equation for Prediction of Three Bond Carbon-Proton Coupling Constants.

13.00 Lunch

14.00 Personal contacts

15.00 P. Sándor,  
DOSY - High Resolution Diffusion Ordered Spectroscopy

15.30 Varian Company Presentation

16.30 Bruker Company Presentation

18.00 Dinner

19.00 Meeting of the NMR Discussion Groups - refreshment sponsored by Bruker and Scientific Instruments Brno

Wednesday April 14, 1999

Morning 8 a.m.

- 8.00 J.Speváček, J.Dybal,  
A Polymer Electrolyte, Poly(ethylene oxide)/LiCF<sub>3</sub>SO<sub>3</sub>, Studied by Solid State <sup>13</sup>C  
NMR and *ab initio* Calculations.
- 8.15 J.Kríz, S.Abbrent, J.Dybal, D.Kurková, J.Lindgren, J.Tegenfeldt, L.Wendsjö,  
NMR Study of Lithium Coordination and Mobility in a Polymer Electrolyte Precursor.

- 8.30 J.Dybal, J.Brus,  
Structure and Morphology of Heterogeneous Polymer Systems Studied by  $^1\text{H}$  Spin Diffusion.
- 8.45 J.Brus,  
 $T_{1\rho}$  ( $^{13}\text{C}$ ) Relaxation at High MAS Speed and Strong Spin Lock Field.
- 9.00 M.Eibl, N.Mundigler, M.Wollerdorfer, H.Weber,  
Investigation of the Structure and Crystallinity of Starch Products by High Resolution  $^{13}\text{C}$  CP/MAS NMR Spectroscopy.
- 9.15 P.Mandal, J. de Ropp, G.N.Lamar,  
Investigation of Substrate Binding Site in Horseradish Peroxidase by Multidimensional NMR.
- 9.30 L.Brecker, D.W.Ribbons,  
Use of  $\text{D}_2\text{O}$  for  $^1\text{H}$  NMR Monitored Biotransformations in  $\text{H}_2\text{O}$ . A Necessary Evil or a Helpful Tool?
- 9.45 V.Veverka, A.Zábranský, I.Pichová, R.Hrabal,  
NMR Studies of 24 kDa Protease from Mason-Pfizer Monkey Virus.
- 10.00 V.Sklenár,  
HCCCH Experiments for Unambiguous Assignments of Thymine Resonances.
- 10.15 R.Fiala, V.Sklenár,  
Multiple-quantum Triple Resonance Experiments for  $^{13}\text{C}/^{15}\text{N}$ -Labeled Nucleic Acids.
- 10.30 R.Fiala, M.Akke,  
 $^{13}\text{C}$  Relaxation Study of Base Dynamics in UUCG and GCAA RNA Hairpin Loops.
- 10.45 L.Trantírek, V.Sklenár,  
Structure Analysis of the  $\text{d}(\text{C}_4\text{G}_4)$  DNA Octamer.
- 11.00 Closing of the Conference