

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

Wednesday April 26, 2000

Afternoon 2 p.m.

- 14:00 Opening of the Conference.
- 14:10 J.Kříž: NMR in local anisotropy; distribution and dynamics of methyl methacrylate sorbed in the shell of a polymer micelle in D<sub>2</sub>O.
- 14:40 R.Hrabal: What is ARIA?
- 14:55 J.Bella, M.Bosco, R.Toffanin, S.Miertuš, S.Paoletti: Conformational analysis of oligosaccharides by <sup>1</sup>H NMR spectroscopy and molecular modelling.
- 15:10 R.Fiala, J.Czernek, V.Sklenář: <sup>13</sup>C chemical shift anisotropy in nucleic acids.
- 15:25 J.Czernek, J.Kvíčala: <sup>19</sup>F shielding in terms of localized molecular orbitals.
- 15:40 V.Proks, M.Holík: Benzylideneanilines – *ab initio* calculation of the solvent dependence of the chemical shift.
- 15:55 M.Holík: Frequent errors made in dynamic NMR spectroscopy.
- 16:10 Break
- 16:40 R.Goc: Computer simulation in analysing NMR results.
- 17:10 E.Kleinpeter, A.Koch: GIAO - HF / DFT calculation of <sup>13</sup>C and <sup>15</sup>N chemical shifts for studying tautomerism and sterically hindered rotations.
- 17:25 L.Brecker, D.W. Ribbons: Enzymic and bacterial culture biotransformations monitored by *in situ* proton-NMR.
- 17:40 Z.Starčuk, Jr., Z.Starčuk, V.Mlynárik, S.Gruber, J.Horký, E.Moser: Adiabatic water suppression for *in vivo* proton MRS.
- 17:55 Z.Starčuk, Jr., Z.Starčuk, V.Mlynárik, S.Gruber, J.Horký, E.Moser: *In vivo* proton MRS: Pulse sequence for simultaneous adiabatic suppression of water and macromolecule resonances.
- 18:10 T.Liptaj, Pham Tran Nghia, K.Burnside-Bromek, D.Uhrín: Determination of residual spin-spin coupling constants in small molecules.
- 19:00 Dinner

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

Thursday	April 27, 2000	Morning 8 a.m.
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- 8:00 C.Seger, R.Pfänder, L.Neumann, M.Zweckstätter, T.A.Holak, R.Tampé: Structure of the active domain of the Herpes Simplex virus protein ICP47 in water/SDS Solution.
- 8:30 P.K.Madhu, P.K.Mandal, R.Grandori, N.Müller: Towards structural constraints in paramagnetic proteins *via* cross-correlation effects.
- 8:45 Z.Klíčová, N.Müller: NMR study of the effect of sorbitol on lysozyme.
- 9:00 N.Müller, P.K.Madhu, P.K.Mandal, R.Grandori, K.Hohenthanner: First NMR investigation of micro-myoglobin.
- 9:15 A.Simon, G.Tóth, H.Duddeck, H.S.M.Soliman, M.H.A.Elgamal: Structure elucidation of novel triterpene saponins.
- 9:30 T.Gáti, G.Tóth, I.Pintér: NMR investigation of the conformation and tautomerism of *bis*- and *tris*-saccharido guanidines.
- 9:45 J.Kovács, G.Tóth, A.Lévai, B.Balázs: Stereochemistry of spiroepoxides obtained by oxidation of 3-arylidene-1-tioflavanones.

10:00 Break

- 10:30 K.E.Kövé, K.Fehér, L.Szilágyi: Band-selective suppression of signals in the 2D NMR spectra of oligosaccharides.
- 10:45 S.Boros, J.Kuszmán, É.Bozó: Structure elucidation of the compounds formed from a 3,4-di-O-methanesulphonyl derivative of glucitol *via* reduction with LAH.
- 11:00 J.Moravcová, A.Hájek, H.Dvořáková, M.Tkadlecová: <sup>1</sup>H NMR Study of the stereochemistry of a xylofuranose with the annelated pyrazolidine ring.
- 11:15 J.Havlíček, M.Hamerníková, Z.Kefurtová, K.Kefurt: Conformational studies of aminodeoxyhexonolactams by <sup>1</sup>H NMR spectroscopy.
- 11:30 E.Kozubek, J.Bohdálková, J.Pavlovský: NMR of humic acids.
- 11:45 J.Tritt-Goc, N.Piślewski, R.Holly: Magnetic Resonance Imaging in Cement.

12:30 Lunch

- 14:00 Yu.F.Oprunenko, D.Yu.Mityuk, A.I.Rebrov, M.M.Stern: Application of multinuclear high resolution, CP-MAS and CRAMPS NMR for the investigation of the structure and dynamic phenomena in transition metal complexes.
- 14:30 D.Kurková, J.Kříž, J.Dybal: NMR study of a cooperative ionic coupling of a polycation with model oligophosphates.
- 14:45 J.Spěvák, L.Hanyková, D.Geschke, M.Ilavský:  $^1\text{H}$  NMR study of phase separation in poly(*N,N*-diethylacrylamide)/ $\text{D}_2\text{O}$  solutions and gels.
- 15:00 J.Brus: Some experimental problems resulting from high speed magic angle spinning of samples.
- 15:15 L.Židek, V.Sklenář: Measurement of residual dipolar couplings in nucleic acids and proteins.
- 15:30 L.Trantírek, M.Urbášek, R.Štefl, V.Sklenář: A method for determining the relative bases orientation in the nucleic acids using dipolar data.
- 15:45 K.Kubíček, L.Trantírek, V.Sklenář: Application of residual dipolar couplings in structural analysis of biomolecules.
- 16:00 Break
- 16:30 R.Marek, R.Fiala, V.Sklenář: Suppression of direct responses in GHMBC and GSQMBC experiments.
- 16:45 J.Sejbal, I.Tišlerová, J.Ježek, J.Vondráček: An NMR and MM conformational study of TN-MAG glycopeptides.
- 17:00 V.Veverka, H.Bauerová, A.Zábranský, I.Pichová, R.Hrabal: Preparation of Mason-Pfizer monkey virus protease for NMR studies.
- 17:15 M.Mazur: Quantity in magnetic resonance spectroscopy - Part 3.
- 17:30 P.Kessler: Information about products of Bruker Analytik GmbH.
- 19:00 Dinner
- 20:00 Meeting of the NMR Discussion Groups - refreshment sponsored by Bruker and Scientific Instruments Brno

- 8:00 E.Kolehmainen, K.Laihia, M.Nissinen, A.Perjéssy, J.Linnato, B.Gautheron, R.Brousier: The origin of the asymmetry of  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of alkyl substituted chlorodicyclopentadienyloxoniobium(V) complexes.
- 8:15 A.Lyčka, D.Micák, J.Holeček, M.Biesemans, R.Willem, J.C.Martins, J.Brus:  $^{119}\text{Sn}$  and  $^{13}\text{C}$  NMR spectra in solution and  $^{119}\text{Sn}$  and  $^{13}\text{C}$  CP/MAS NMR spectra of bis(tributyl)tin(IV) and dibutyltin(IV) L-(+)-ascorbates and 5,6-isopropylidene L-(+)-ascorbates.
- 8:30 A.Růžička, R.Jambor, J.Holeček, A.Lyčka, M.Biesemans, R.Willem, J.C.Martins: The NMR study of Intramolecular Coordination in Organometallic Compounds
- 8:45 T.Lébl, D.Steinborn, J.Holeček, M.Dymák: Protodemallation of 2-functionalised vinylstannanes -  $^1\text{H}$  NMR kinetic measurement.
- 9:00 A.Popkov, P.A.Manorik, T.Weidlich: Role of an apical  $\eta_2$ -ligand in long-range  $^nJ(^{13}\text{C}, ^{13}\text{C})$ ,  $^nJ(^{15}\text{N}, ^{13}\text{C})$  and  $^nJ(^{15}\text{N}, ^{15}\text{N})$  interactions in square-pyramidal nickel complex of Schiff base of of (*S*)-2-(*N*-benzylpropyl)-aminobenzophenone and  $^{15}\text{N}$ ,  $1\text{-}^{13}\text{C}$  or  $2\text{-}^{13}\text{C}$ -labelled glycine.
- 9:15 P.Sedmera, V. Křen, J.Ulrychová, V.Šimánek, D. Stevenson, V.Přikrylová, P.Halada, P.Kosina: NMR Studies of Flavolignans.
- 9:30 P.Kačer, A.Marhoul, M.Kuzma, L.Červený: NMR Analysis of Alkylcyclohexanols.
- 9:45 H.Dvořáková, J.Vlach, J.Lang, J.Sýkora, P.Lhoták, R.Hrabal: Conformational characteristics of partially O-alkylated thiacalix[4]arenes
- 10:00 E.Kozubek, A.Wolf, P.Sikora: NMR, GC, GC/MS composition studies of the fossil fuels liquid derivatives.

11:00 Closing of the Conference