International Conference on Natural Products and Physiologically Active Substances (ICNPAS-2004)
September 12-17, 2004, Novosibirsk, Russia
Oral Communication

Potentials of Modern Mass Spectrometry in Structure Elucidation of Natural Products

Jasna Peter-Katalinić

Institute for Medical Physics and Biophysics, Biomedical Analysis Group, University of Münster, Robert-Koch-Str. 31, 48149 Münster, Germany
e-mail: jkp@uni-muenster.de

Mass spectrometry (MS) is a powerful analytical technique for identification of unknown compounds by determination of mass-to-charge (m/z) values of intact molecular ions and their fragments. Mass spectra, reflecting physical and chemical properties of the analytes, provide qualitative and quantitative data for structure determination of synthetic low and high molecular compounds and for the wide diversity of natural compounds. Besides, the high sensitivity and accuracy of MS techniques offer high potential for forensic and environmental sciences. Current applications to medicine involve direct screening of protein profiles in human plasma and urine, and of drugs and their metabolites in body fluids. Exploratory strategies, developed for genomics and proteomics, serve for identification of expression profiles in human health and disease.

Using soft ionization techniques, introduced 25 years ago to MS, it became possible to ionize polar molecules without thermal evaporation. Fast Atom Bombardment (FAB) ionization has been successfully and generally applied to analysis of different class of compounds, like peptides, oligosaccharides, oligonucleotides, or plant glycosides [1]. Modern soft ionization methods are Electrospray Ionization (ESI) and Matrix Assisted Laser Desorption/Ionization (MALDI), which are broadly used for detection of low and high molecular weight compounds containing polar functional groups. Depending on the type and and technical characteristics of instruments, experiments for identification by detection of the molecular ion and for the tandem mass spectrometry experiments to induce formation of diagnostic fragment ions, can be designed in different ways.

In this lecture structural elucidation of plant saponins [2], bacterial cardiolipins [3], O-linked glycopeptides from human mucine [4] and from viruses [5], intact proteins from thermophilic bacteria [6], glycolipids from human neutrophils [7] and from human brain [8] by ESI Quadrupole-time-of flight (QTOF) and ESI Fourier Transform Ion Cyclotron Resonance (FT-ICR) MS at 9.4 T will be presented. Advantages beneficial for structural determination of natural compounds, a combination of high resolution and high mass determination accuracy for identification of single components in complex mixtures will be illustrated and discussed.

References:

[1] J. Peter-Katalinić, Mass Spectrom. Rev. **1994**, 13, 77-98; [2] S.-J. Guo, J. Peter-Katalinić, L. He, D.-L.Cheng, Pharmazie **1998**, 53, 481-485; [3] A. I. Beckedorf, C. Schäffer, P. Messner, J. Peter-Katalinić, J. Mass Spectrom. **2002**, 37, 1086-1094; [4] F.-G. Hanisch, S. Müller, H. Hassan, H. Clausen, N. Zachara, A. A. Gooley, H. Paulsen, K. Alving, J. Peter-Katalinić, J. Biol. Chem. **1999**, 274, 9946-9954; [5] S. Schmitt, D. Glebe, K. Alving, T.K. Tolle, M. Lindner, H. Geyer, D. Lindner, J. Peter-Katalinić, W.H. Gerlich, R. Geyer, J. Biol. Chem. **1999**, 274, 11945-11957; [6] K. Strupat, D. Šagi, H. Bönisch, G. Schäfer, J. Peter-Katalinić, The Analyst **2000**, 125, 563-567; [7] W. Metelmann, J. Müthing, J. Peter-Katalinić,Rapid Comm. Mass Spectrom. **2000**, 14, 543-550; [8] W. Metelmann, Ž. Vukelić, J. Peter-Katalinić, J. Mass Spectrom. **2001**, 36, 21-29;