

# **Elucidation of the complex molecular structure of wheat straw lignin polymer by atmospheric pressure-photoionization-quadrupole-time-of-flight tandem mass spectrometry**

**Joseph H. Banoub**

Department of Chemistry, Memorial University of Newfoundland, and  
Fisheries and Oceans Canada, Science Branch, Special Projects, P.O. Box 5667, St.  
John's, Newfoundland, A1C 5X1, Canada

Wheat straw lignin was extracted using the novel AVIDEL, procedure that selectively separates the cellulose, hemicelluloses and lignin. Atmospheric Pressure PhotoIonization Mass spectrometry (APPI-MS) has proven to be powerful analytical tool capable of ionizing small to large lignin oligomers, which cannot be ionized efficiently by APCI and ESI. The APPI-MS of the extracted wheat straw lignin were recorded in the positive and negative ion modes. The positive mode APPI-MS indicated the exact presence of **39** specific oligomeric ions. The APPI-MS recorded in the negative mode, indicated the additional presence of at least **18** specific oligomeric ions.

The structural characterization of this novel and complete series of **57** specific related oligomers, was achieved by calculating the exact molecular masses measured with the high resolution QqToF-MS. There were identical oligomeric species that photoionized in both the positive and negative ion modes, which formed the respective protonated and deprotonated molecules. Low energy collision tandem mass spectrometric analyses performed with a QqToF-MS/MS hybrid instrument provided unique dissociation patterns of the complete series of novel precursor ions. These MS/MS analyses provided diagnostic product ions, which assisted us to expose the exact molecular structure and arrangement of the selected different **57** related ionic species.