EuroSciCon

EuroSciCon Conference on

Biochemical, Chemical Engineering & Mass Spectrometry

November 19-20, 2018
Prague, Czech Republic

Arch Chem 2018, Volume: 2
DOI: 10.21767/2572-4657-C4-012

# ELECTROSPRAY IONIZATION WITH HIGH-RESOLUTION MASS SPECTROMETRY AS A TOOL FOR LIGNOMICS, WITH AND WITHOUT SEPARATION BY MW

**Evguenii I Kozliak, Anastasia A Andrianova, Joshua Hatton, Thomas DiProspero, Clayton Geib, Angel Ugrinov, Mukund Sibi, Irina P Smoliakova and Alena Kubátová**

University of North Dakota, USA

**Both lignin and its degradation products are notoriously difficult to characterize, due to lignin's irregular heteropolymeric nature. We have developed a method based on electrospray ionization high-resolution time-of-flight mass spectrometry (ESI-HR TOF-MS) to expand the lignomics toolkit while targeting the simultaneous detection of low and high molecular weight (MW) lignin species. The effect of a broad range of electrolytes and various ionization conditions on ion formation and ionization effectiveness was studied using a suite of mono-, di- and triarene lignin model compounds as well as Kraft alkali lignin. Contrary to the previous studies, the positive ionization mode was found to be more effective for methoxy-substituted arenes and polyphenols, i.e., species of a broadly varied MW structurally similar to the native lignin. For the first time, we are reporting formation and deconvolution of lignin multiply charged species in the presence of 100 mmolL-1 formic acid in the positive ESI mode. The developed method enabled the detection of lignin species with an MW between 150 and 9,000 Da or higher, depending on the mass analyzer. The obtained $M_n$ and $M_w$ values of 1,500 and 2,500 Da, respectively, were in good agreement with those determined by size exclusion chromatography. Furthermore, the deconvoluted ESI mass spectrum was similar to that obtained with matrix-assisted laser desorption/ionization (MALDI)-HR TOF-MS, but MALDI featured a higher signal-to-noise ratio. The formation of multiply charged species was confirmed with ion mobility ESI-HR Q-TOF-MS. These results were further confirmed by, successful lignin fractionation by size exclusion chromatography into four fractions, with calculated Mn values 9,980 Da, 3,150 Da, 1,330 Da, and 1,210 Da, respectively.**

evguenii.kozliak@und.edu