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C_{60} Secondary Ion FT-ICR Mass Spectrometry: High Mass Resolving Power and High Mass Accuracy SIMS

Ljiljana Paša-Tolić,[1] Donald F. Smith,[2] Franklin E. Leach III,[1] Errol W. Robinson,[1] and Ron M.A. Heeren[2]

[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA, USA
[2]FOM Institute AMOLF, Biomolecular Imaging Mass Spectrometry, Amsterdam, The Netherlands

Mass spectrometry imaging is a powerful tool for chemical imaging of complex biological surfaces. Most MS imaging workflows employs MALDI, which is typically used to image drugs/metabolites and biomolecules directly from biological surfaces. However, the spatial resolution of MALDI is typically limited by the laser spot focus; whereas secondary ion mass spectrometry (SIMS) has long been used for sub-micrometer imaging of organic and inorganic surfaces. Polyatomic primary-ion sources (Au/Bi clusters and C_{60} (buckminsterfullerene) provide improved sensitivity for SIMS imaging of biological surfaces. SIMS is typically coupled to a time-of-flight (TOF) mass analyzer for high sensitivity due to the low number of secondary ions produced. However, they lack mass resolving power and mass accuracy for high specificity chemical imaging. Recently, we have reported the first coupling of a polyatomic C_{60} primary ion gun with a Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS) [1]. Here, we will discuss the motivation, design and implementation of this platform, which provides high mass resolving power ($m/\Delta m_{50\%}$ > 100,000), high mass accuracy (< 1 part-per-million, ppm) and tandem MS capabilities.

A 40 keV electron-impact based C_{60} primary ion gun was interfaced to a 12 T Bruker solariX FT-ICR mass spectrometer. A schematic of the source is shown in Figure 1. Secondary ions are collected by an optimized RF only octopole and transferred into the commercial FT-ICR via two RF only quadrupoles. The C_{60} gun is operated in direct-current mode for optimum FT-ICR MS spectral performance. Secondary ions directly from biological tissue sections can be subjected to collision induced dissociation and yield fragment ions which can be assigned unique elemental compositions, leading to parent ion identification. On tissue MS imaging experiments yield hundreds of tissue specific ions, many of which cannot be resolved on lower performance mass spectrometers.

High mass resolving power ($m/\Delta m_{50\%}$ > 100,000) secondary ion FT-ICR MS is demonstrated on standards as well as mouse brain biological tissue sections. Measured mass accuracy of 1 ppm or better have been achieved in the tissue imaging modality as shown in Figure 2. Collision induced dissociation is shown for ions directly from tissue sections. Further, MS imaging at 40 μm spatial resolution has been achieved. Tissue imaging of brain and heart sections yields rich mass spectra with hundreds of well-resolved secondary ions. Progress towards ultra-high mass resolving power SIMS and improved MS imaging sensitivity will be discussed [2].

References:

[1] DF Smith, *et al*, Analytical Chemistry **83** (2011), p. 9552.
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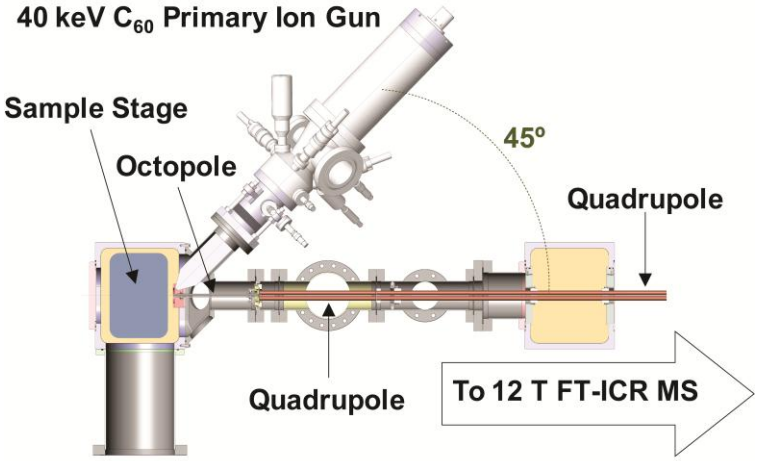

Figure 1. Schematic representation of the C_{60} ion source that has been mated to FT-ICR MS.

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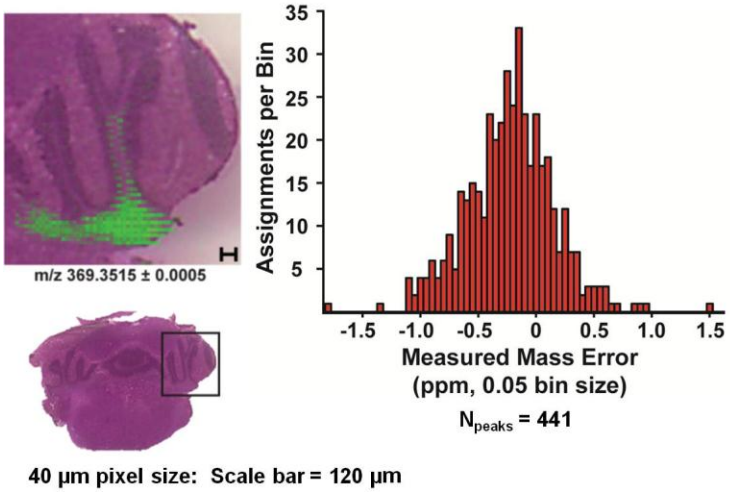

Figure 2. C_{60} secondary ion FT-ICR MS tissue imaging with high mass accuracy.

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