MASS ACCURACY OF MULTI-REFLECTING TOFMS

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Analytical chemistry becomes more and more alert of the importance of mass accuracy in mass spectral measurements. With development of new data processing algorithms, true specificity and the separation power of mass spectral measurements is primarily limited by mass accuracy rather than by the resolving power. Sub-ppm mass accuracy is desired in proteomics for reduced number of incorrect identifications (an increase in the confidence of hits) and it would extend the mass range and the elemental diversity of compound identification in other areas of mass spectral analyses. As demonstrated on GCxGC-MS case [1], the separation capacity of hybrid separation methods improves with mass accuracy. As been shown in [2], accurate mass defects, in-large, correlate with mobility shifts and in this sense precise mass measurements duplicate the mobility separations. Currently, commercial high-resolution instruments –time-of-flight MS, ICR FTMS and electrostatic traps – are just approaching a barrier of sub-ppm mass accuracy. Back in 2006, multi-reflecting time-of-flight mass spectrometers (MR-TOF) were demonstrated to reach 1 Million resolving power [3] for a narrow mass range. At full mass range, the resolving power R is limited by the instrument size with typical R=200,000 to 300,000 [4], meaning that mass spectral peaks are 3-5ppm wide. With detected ion fluxes up to 1E+8ion/s, ion statistics potentially allows reaching low 1ppb mass scatter at sub second spectral acquisition. However, the true mass accuracy with internal calibration still remains in the order of 0.1ppm (i.e. 100ppb). The presentation will discuss several already recognized limiting factors: In-spectra ion statistical limit, limiting mass accuracy at low intensity signals or at fast spectral acquisitions; diversity of not fully resolved isobars from chemical background systematic curvature and oscillations of mass calibration curve, produced by finite rise time and oscillations induced on accelerator electrodes: Slow drifts and higher frequency noise of power supplies; Mass and charge dependent parameters of ion beam in front of MRTOF; Effects of nanoampere currents within interfaces; Space charge effects within analyzers and Noise and saturation of the data system. Most of those factors can be avoided or at least accurately recognized for producing reliable measurement results.

References

1. Verenchikov et. al, IMSC 2014, MOS01-05

2. Kozlov ey.al, ASMS 2014

3. Verenchikov et.al, Technical Physics, Vol. 50, No. 1, 2005, pp. 82–86.

4. Verenchikov et.al, JASCM, 2017, 6, 1-22.

BIOGRAPHY

Anatoly Verenchikov is currently the Director of "Mass Spectrometry Consulting Ltd." Bar, Montenegro and served as the Founder for the company from 2007-2016. In 2015, he received the golden medal from the Russian Society of Mass Spectrometry for outstanding achievements in mass spectrometry, Moscow, Russia. He also received the Golden award of Pittsburg Conference for Pegasus MRTOF, USA in 2011. He is the author of over 50 patents, more than 200 papers and conference presentations.

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