

Project A49

OrbiSIMS Metrology: Linearity of the Intensity Scale and Implications to Data Processing

Objectives

The previous VAMAS TWA 2 A37 project evaluated a comparison metric for Orbitrap Secondary Ion Mass Spectrometry (OrbiSIMS) instruments [1]. Participant data enabled assessment of repeatability, reproducibility and noise characteristics. However, the data was very rich, and further evaluation is anticipated to yield a basis for standardised advanced data analysis corrections of artefacts arising from non-linearities [2]. Project A49 will focus on analysing existing data from A37 and welcomes new contributions from other laboratories not involved in the original study. We will conduct this under TWA 2 stream 4: Data workflow, methods and best practice (DAT).

Background

In OrbiSIMS [1], a quasi-continuous stream of secondary ions is injected into a special ion trap where they revolve around a central spindle shaped electrode and oscillate along it with a frequency inversely proportional to the square root of the mass of the ion. An image charge is created in a pair of outer electrodes and is measured with time using a differential amplifier. The time-domain transient signal is digitised and can be converted to the frequency (and hence mass) domain by a Fourier transform.

Standardization Needs

With a growing global number of OrbiSIMS instruments there is an increased need for reproducible and intercomparable measurements. The methods of this project can be used for internal quality control, and improved reproducibility is directly beneficial for industries that use the technology such as Semiconductors, Pharmaceuticals, Printed electronics, Organic electronics, and Energy storage.

Work Programme

For this study, we will assess the linearity of the signal intensity scale. The experiments consist in systematically varying the number of secondary ions sent to the Orbitrap. Preliminary studies found that non-linearity in signal arises from space-charge effects in the trap and is m/z -dependant. These findings have direct implication on applications such as depth profiling and imaging.

Statistical analysis of the results from participants will be conducted as consistent with ISO/TS 11308.

Funding

Participants fund their own involvement in the project.

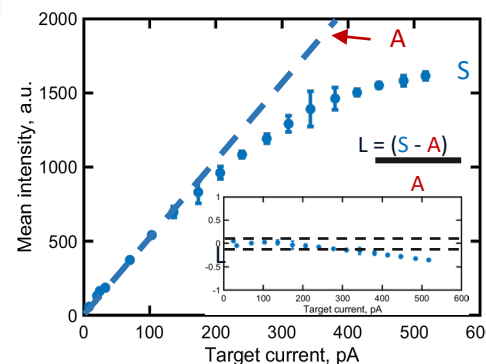


Figure 1: The experiment to measure the linearity the intensity scale requires a systematic variation of the number of secondary ions into the Orbitrap. Linearity (L) is calculated based on the deviation against linear prediction of each m/z signal in function of total intensity.

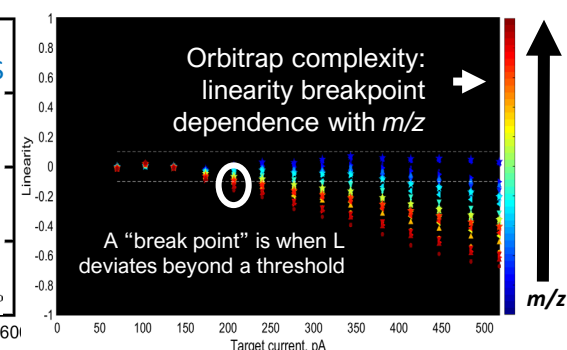
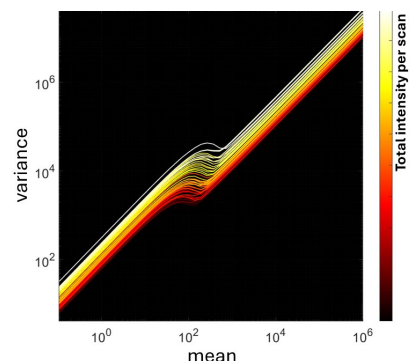


Figure 2: We previously introduced the WSoR model [2] for OrbiSIMS data. A comparison of WSoR models across intensity regimes showed a dependence of the variance overall with the total intensity per scan in the Orbitrap analyser.



Deliverables and Dissemination

- A VAMAS report on the interlaboratory comparison.
- A peer-reviewed article describing the results of the intercomparison study.
- A presentation at a specialists conference/meeting

References

- [1] Passarelli *et al. Nat Methods* **2017**, 14(12), 1175-1183. doi: 10.1038/nmeth.4504
 [2] Keenan *et al. Nat. Commun.* **2025**, 16(1), 6398.

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