

Using the Advion TriVersa NanoMate® for rapid analyte identification based on static nESI-MS/MS (Infusion MS/MS) employing polarity switching experiments

Introduction

Automated static nano-ESI-MS/MS (Infusion MS/MS) is an easy-to-use and high throughput approach to analyte identification. It is particularly useful in the field of shotgun lipidomics, which itself has great potential for biomarker discovery and gained some significant attention in the last couple of years [Schuhmann et al. 2012; Jung et al. 2011; Han et al. 2011].

In order to simplify shotgun lipidomic approaches even further, the TriVersa NanoMate can now change nano-ESI spray polarity within the same Infusion experiment (Figure 1).

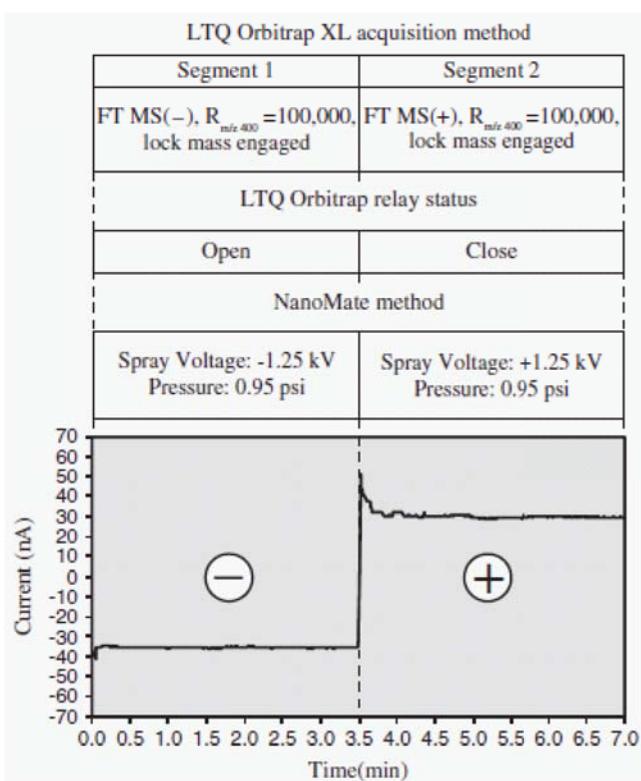


Figure 1: Example of the experimental set-up to run shotgun lipidomics samples using the Advion TriVersa NanoMate with polarity switching [Schuhmann et al.].

- New TriVersa NanoMate firmware allows polarity switching within the infusion run
- <10 min run time for comprehensive shotgun lipidomics
- No carry-over due to one sample one tip one sprayer strategy
- High throughput analysis

Using both positive and negative MS datasets in one run, researchers from Andrej Shevchanko's lab found that: '...For each sample in both positive and negative mode, FT MS (and if required, many MS/MS) spectra could be acquired in rapid succession within the same noninterrupted sequence. Neither throughput nor sensitivity was compromised, while lipid identification specificity and coverage of lipid classes were markedly improved....' [cited from Schuhmann et al. 2012].

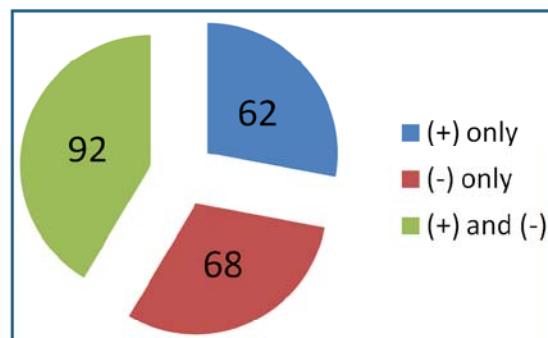
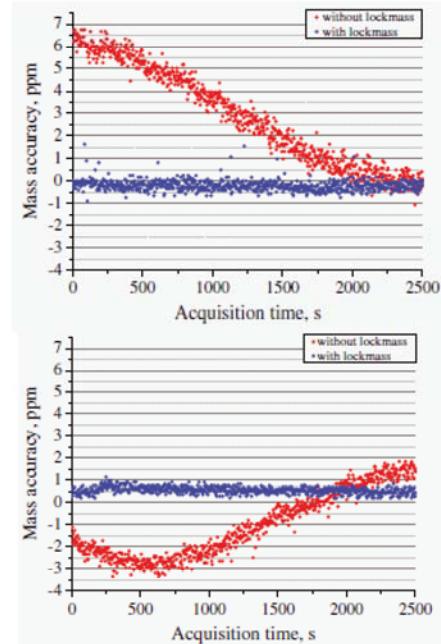


Figure 2: +/- polarity switching shows advantages in lipid coverage, example shown from a bovine heart extract showing a 75% increase in lipid identification comparing to positive ion mode alone and 16% increase comparing to negative polarity only [Schuhmann et al.].

Using Lock masses to compensate for mass drifts after polarity switches

Polarity switching in either a rapid, alternating way or in a static approach always causes temporary changes in the detector electronics. These significantly affect mass accuracy in higher resolution instruments such as Tofs, FTs or Orbitraps due to time dependant mass shifts. A suitable way to compensate for these effects is the use of lock masses [Olsen et al. 2005]. As demonstrated by Schuhmann et al. 2012, lock masses can be used to maintain sub 1 ppm mass accuracy when triggering a polarity change, otherwise causing off-setts of up to 7 ppm (Figure 2).

Figure 2: Mass accuracy of a single analyte over time after the polarity switch from negative to positive (top) and positive to negative polarity (bottom), with lock mass use (blue) and without (red) [Schuhmann et al. 2012].



TriVersa NanoMate set up for polarity switching experiments

A firmware upgrade allows the TriVersa NanoMate to be used for a polarity switching experiment by using Rel3 as an input/output signal reader that internally switches the spray polarity as well [Schuhmann et al. 2012, Advion Technical Bulletin TB_NMT014_RevA_2012].

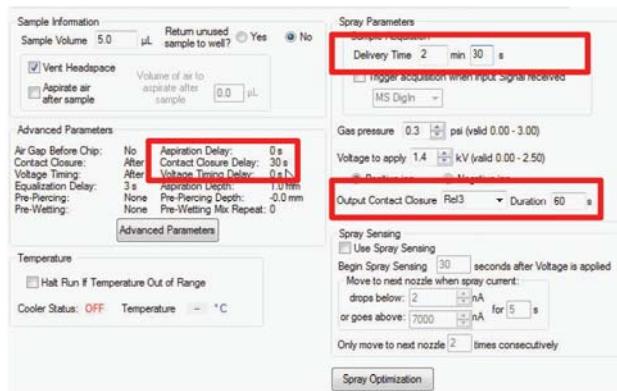


Figure 4: Software settings in ChipSoft to allow polarity switching experiments.

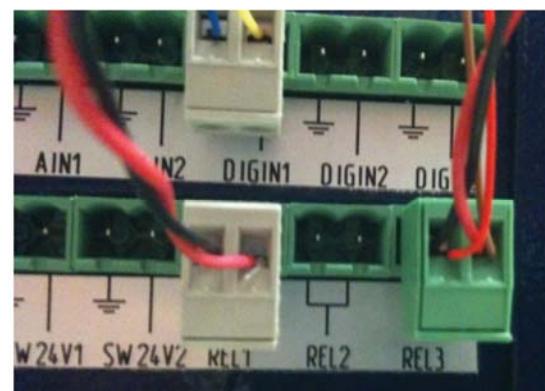


Figure 3: Simple hardware set-up to allow the TriVersa NanoMate to run polarity switching experiments.

References

- [1] Schuhmann K, Almeida R, Baumert M, Herzog R, Bornstein SR, Shevchenko A.: Shotgun lipidomics on a LTQ Orbitrap mass spectrometer by successive switching between acquisition polarity modes. *Journal of Mass Spectrometry* 2012; 47(1): 96-104.
- [2] Han X, Yang K, Gross RW: Multi-dimensional mass spectrometry based shotgun lipidomics and novel strategies for lipidomic analyses. *Mass Spectrometry Reviews* 2012; 31(1):134-78
- [3] Jung HR, Sylvanne T, Koistinen KM, Tarasov K, Kauhanen D, Ekroos K: High throughput quantitative molecular lipidomics. *Biochimica and Biophysica Acta* 2011, 1811 (11), 925-934.
- [4] Olsen JV, de Godoy LM, Li G, Macek B, Mortensen P, Pesch R, Makarov A, Lange O, Horning S, Mann M: Parts per million mass accuracy on an orbitrap mass spectrometer via lock-mass injection into a C-trap. *Molecular and Cellular Proteomics* 2005; 4(12): 2010-2021.
- [5] Advion Technical Bulletin: TB_NMT014_RevA 2012