Impact of different optical lenses while using the LA-REIMS imaging setup

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Introduction

- Laser Assisted Rapid Evaporative Ionization Mass Spectrometry (LA-REIMS) is an ambient technique requiring no sample preparation
- We have previously demonstrated on veterinary sections that LA-REIMS can be used as an alternative imaging technique for tissue distinction through micro-scale resolution metabolic profiling [1]
- During the optimization of the system, we found that several hardware components affect the laser beam and change the obtained mass spectra

[1] waters.com/posters:
Fully Automated Chemical Imaging with LA-REIMS

Aim

Investigate the effect of different optical lenses in terms of focal length, lens diameter, material, and energy density on the resulting mass spectra.

Experimental

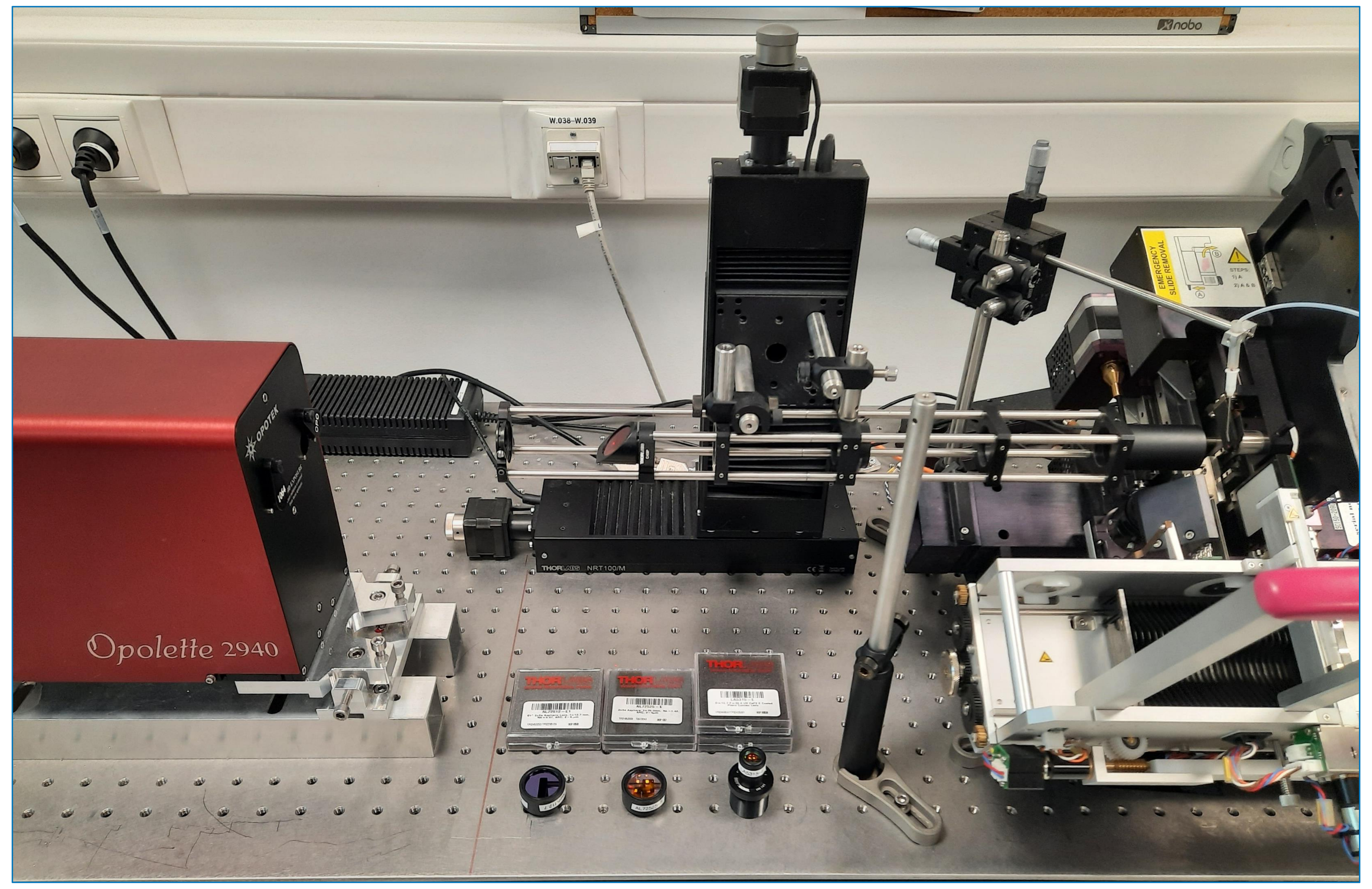

Figure 1. LA-REIMS™ imaging setup

- Optical parametric oscillator used on 2940 nm
- Generated aerosol transferred into Xevo™ G2-QTof-MS equipped with REIMS™ source
- Tested lenses: aspheric (a,) ZnSe or plano convex (p.c.) CaF_2

Results

- Ø 1 in a. ZnSe (f = 12.7 mm) 6.02 J/cm^2
- Ø 1 in a. ZnSe (f = 12.7 mm) 4.47 J/cm^2
- Ø 1 in a. ZnSe (f = 12.7 mm) 3.31 J/cm^2
- Ø 1 in a. ZnSe (f = 12.7 mm) 1.15 J/cm^2
- Ø 1 in a. ZnSe (f = 25 mm) 3.25 J/cm^2
- Ø ½ in p. c. CaF_2 (f = 20 mm) 3.12 J/cm^2
- 2x Ø ½ in p. c. CaF_2 (f = 6 mm) 2.56 J/cm^2

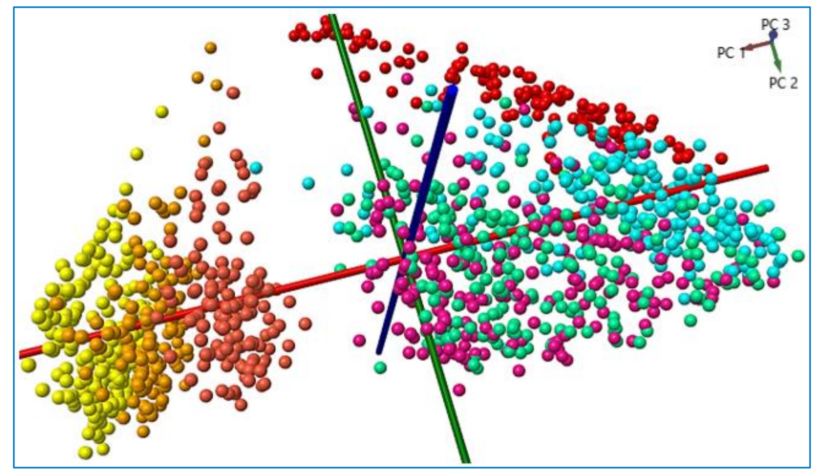

Figure 2. PCA model of the same homogenous pork liver measured with different optical lenses

- Actual energy densities are calculated through the obtained spot sizes and are listed to their corresponding color in the legend on the left
- Every measured lens setup showed a visible shift in the PCA model between the groups

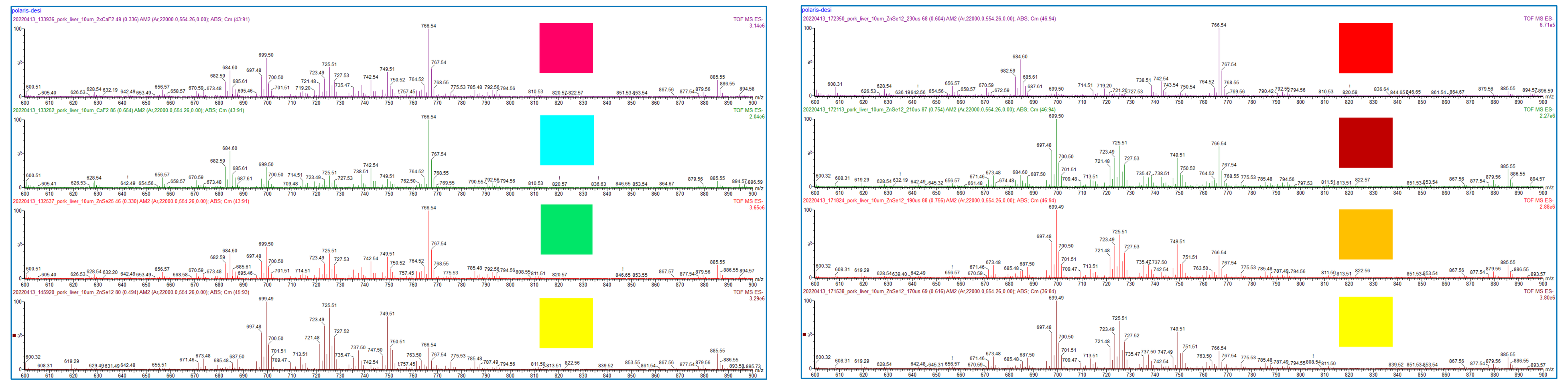

Figure 3. Combined spectra of 50 scans from each measurement (Differing lenses on the left, same ZnSe lens on different energy settings on the right)

- A connection of the following peak-pairs was detected: 725.5 m/z and 742.5 m/z as well as 749.5 m/z and 766.5 m/z

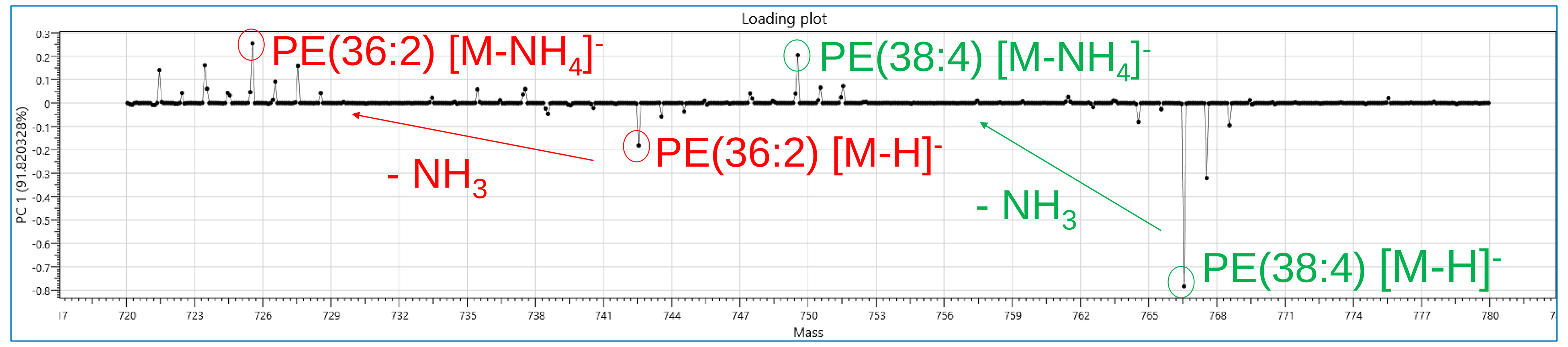

Figure 4. PC 1 Loading plot from 720-780 m/z

- PC 1 Loading plot represents the most significant peak pair differences in the model (same peaks as in Figure 3)
- Based on fragmented ion spectra the peak-pairs were identified as PE(36:2) and PE(38:4) associated with ammonia loss.

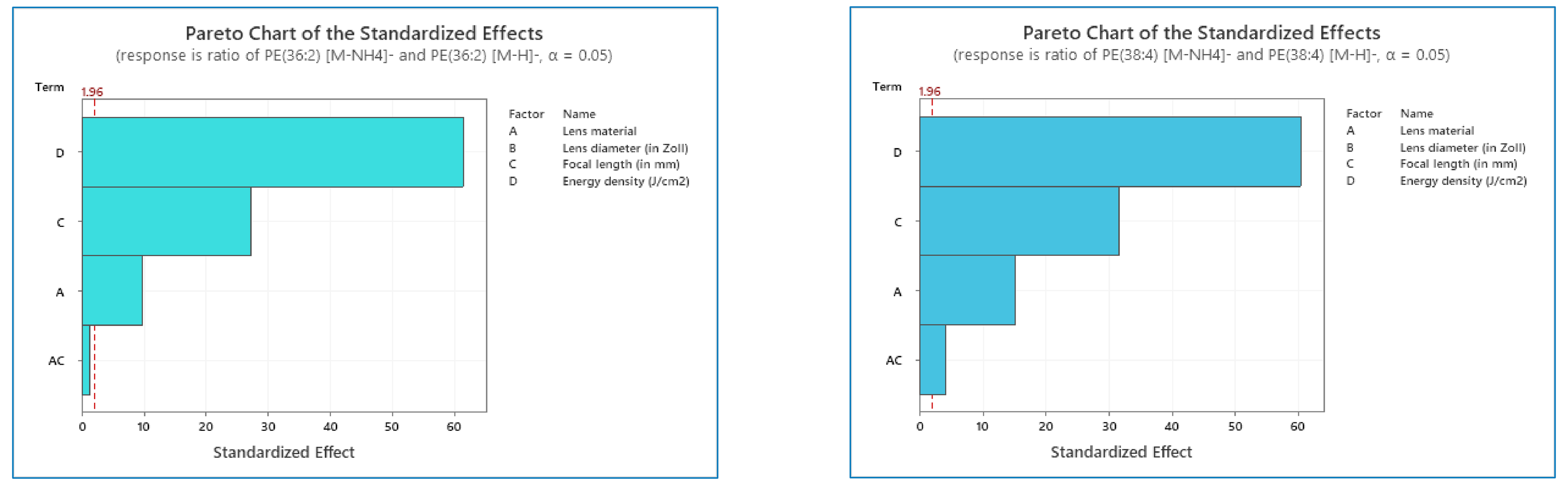

Figure 5. Pareto charts showing the impact of standardized effects on the peak pair ratios

- Pareto charts confirm that the effect of energy density has the most influence on the peak-pair ratio change
- The achieved spot size depends also on lens material and focal length, which also influence the energy density and leads to further changes of the ratios

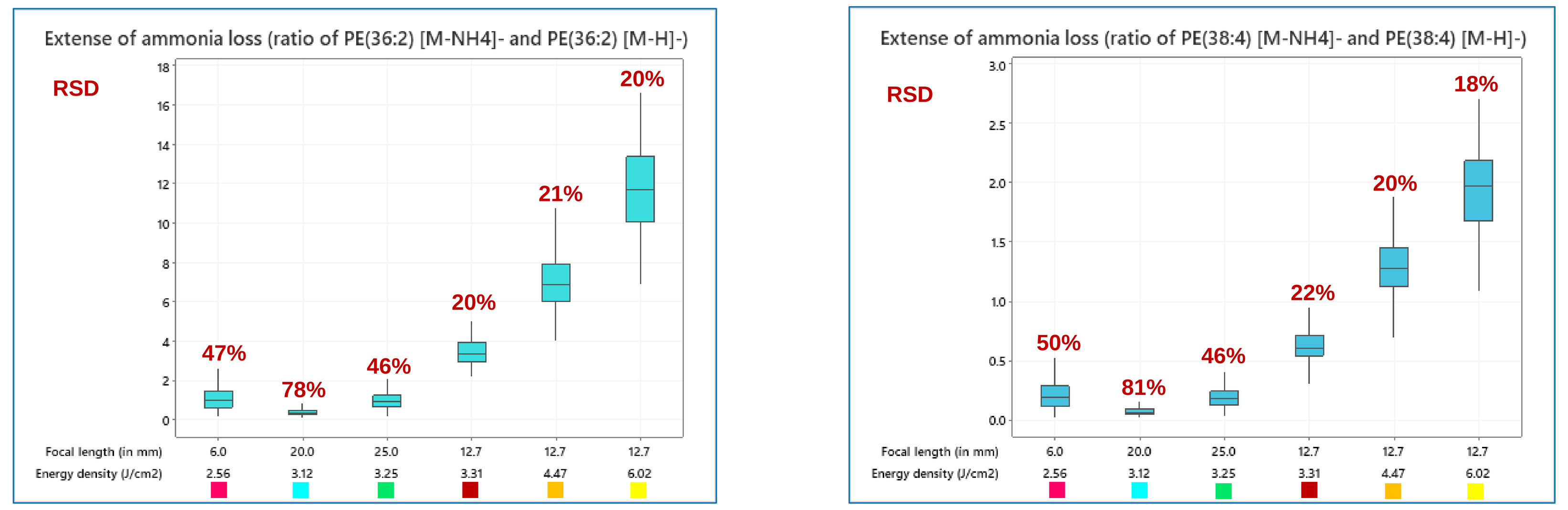

Figure 6. Boxplots representing lens focal length and energy density (as most important effects) against intensity ratio of PE(36:2) [M-NH$_4$]$^-$ and PE(36:2) [M-H]$^-$ on the left and PE(38:4) [M-NH$_4$]$^-$ and PE(38:4) [M-H]$^-$ on the right and included relative standard deviation (RSD)

- Observing within a lens (ZnSe), a more pronounced ammonia loss is visible at higher energies, increasing the variance of the peak ratios
- Focal length dependence visible through the increased ratio variance from the violet measurement despite lower energy density
- RSD showing the robustness of high energy density measurements

Conclusion

- Spectral differences between lens setups have been discovered
- Ammonia loss was determined to be the cause of the spectral differences; the higher the energy density, the higher the ammonia loss
- To explore this in more detail, a beam profile needs to be created from each tested lens to see the exact energy impact on the sample and define, what the actual real spot size is.

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