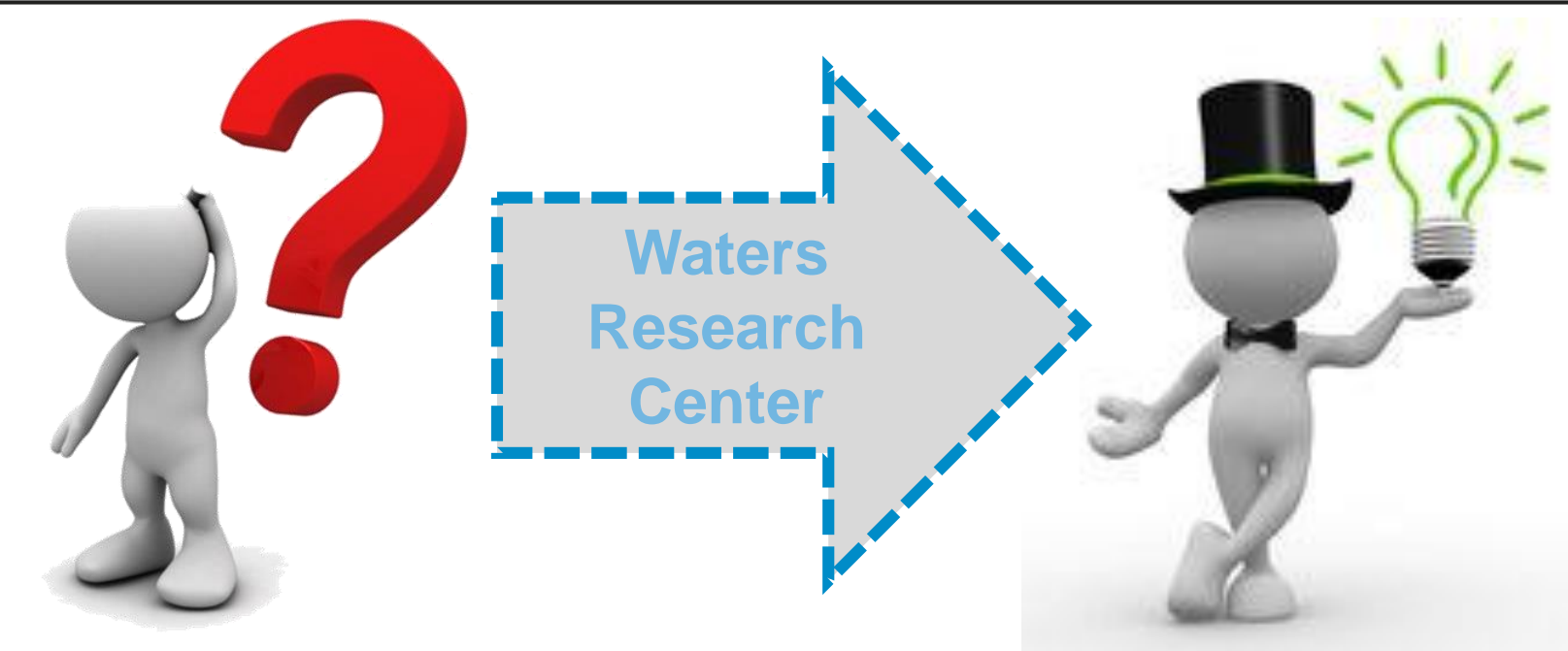


# QUALITY CONTROL ASPECTS OF REIMS TECHNOLOGY

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Is your Ambient MS quality controlled?

Are you suffering from insufficient reproducibility?



**Solution: REIMS**

## INTRODUCTION

- Rapid Evaporative Ionization Mass Spectrometry (REIMS)** is a quick and efficient method for profiling complex biological samples such as tissues, microbial samples or food products without the time consuming sample preparation steps.
- However, to date no quality control protocol for REIMS has been published.
- First** a system suitability method and sample was developed to allow us to **routinely determine the instrument system status**.
- Secondly**, data was collected from various types of REIMS sources over a period of **2.5 years** using certified standards, commercially available **longtermly consistent materials** and **biological samples** to verify the reliability, accuracy and precision of REIMS.

## METHODS

Study	Quality Control Application	Long-term Reproducibility
Samples	Standard phosphatidylglycerols (DPPG, POPG, DOPG, DSPG)	Bovine liver and muscle Certified meat homogenate Chocolates (75% & 90% cocoa)

- Ablation:** The REIMS technology is based on the direct analysis of the aerosol generated by an ablation source (OPO laser, CO2 laser, commercially available and custom-built RF generators). To remove or reduce user introduced variability robotic handling systems were used.
- Detection:** The generated aerosol was introduced into the REIMS source on a Waters Xevo G2-XS ToF MS and spectra were acquired in negative ion mode over the mass/charge range 50-1200. Lockmassed to leucine enkephalin.(554.2615 m/z)
- Data evaluation:** The data was processed using multivariate statistical algorithms including **Principal Component Analysis (PCA)** and **Linear Discriminant Analysis (LDA)** to describe the spectral set characteristics and to build a sample classifier.

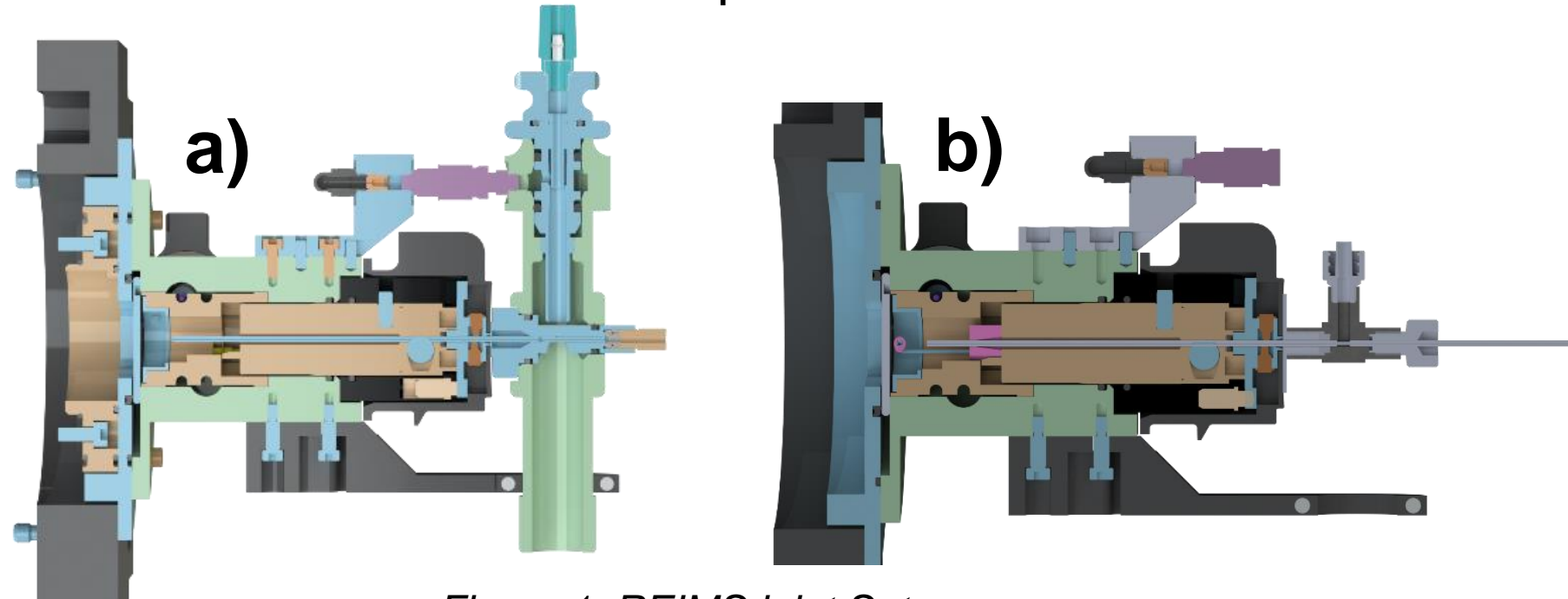
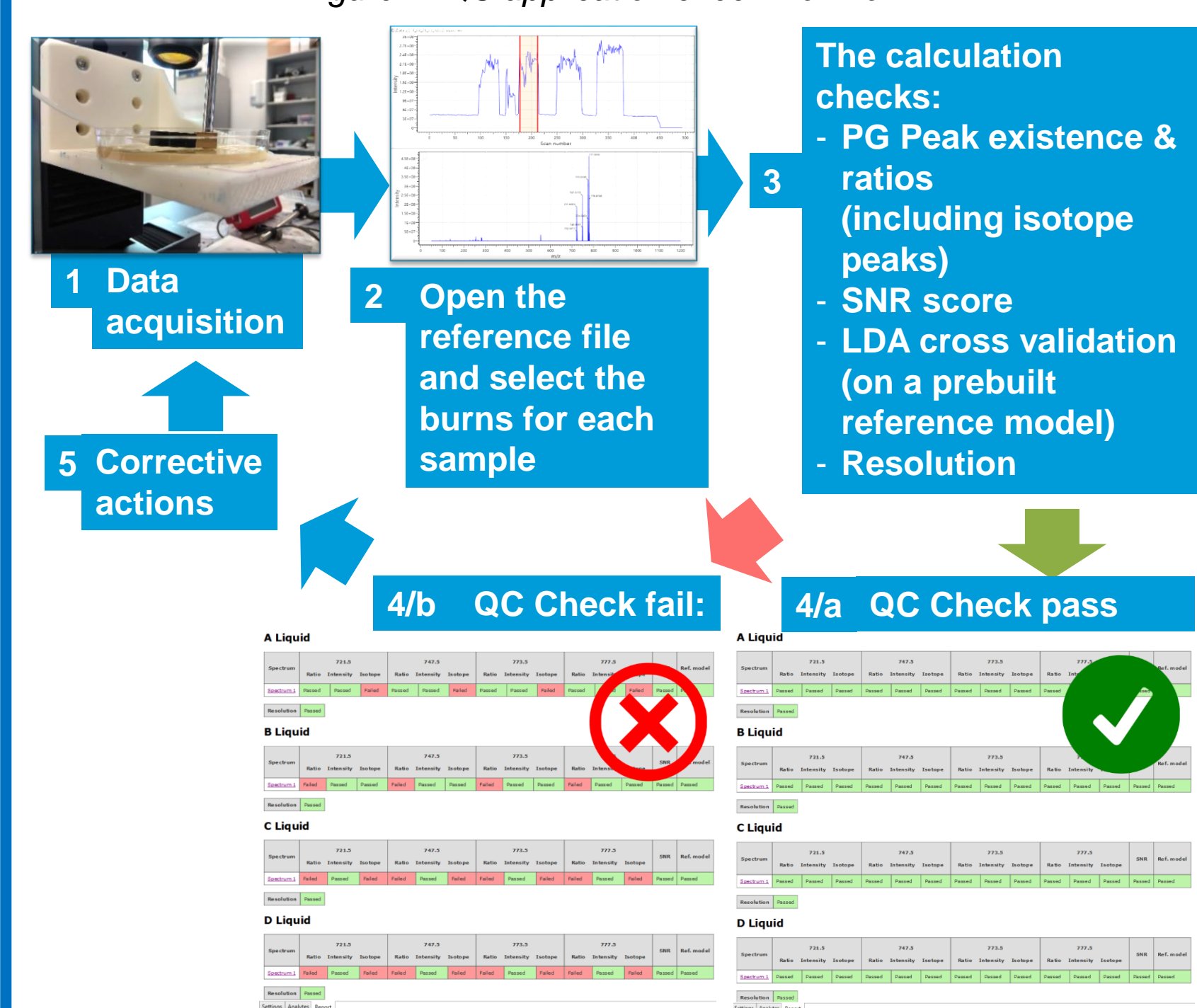


Figure 1: REIMS inlet Setups:

a)Traditional Venturi b) Direct-T ( use when the smoke generation is less than 40ug/sec)

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Figure 2: QC application check workflow



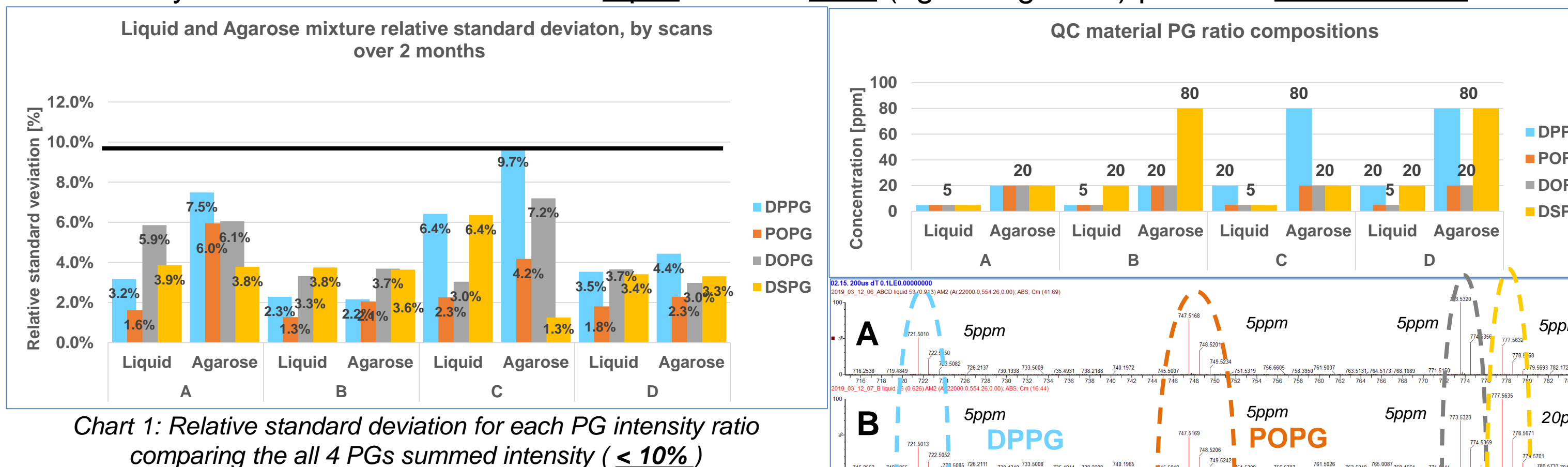
Spectrum	Ratio	Intensity	Isotope	Ratio	Intensity	Isotope	Ratio	Intensity	Isotope	Ratio	Intensity	Isotope	SNR	Ref. model	
721.5	38	100000	74.4	105.5	722.5	42	11760.33	747.5	18	100000	7.4	105	748.5	45	11193.93
773.5	24	100000	13.8	197	774.5	47	14217.43	777.5	21	100000	31.4	1619	778.5	47	16898.87

**Summary:**  
A quality control **software** and reference **material** for REIMS technique was developed, which is applicable to **system suitability testing**.

To provide the users a **quality checking application** for the **Rapid Evaporative Ionization Mass Spectrometry (REIMS)**, including a standardized material and a software

## RESULTS QUALITY CONTROL APPLICATION

- 4 different mixture of 4 different PG standards were used to formulate the QC control materials
- Thermal ablation has been done with **OPO laser** on a **moving stage** [30mW, 1mm/sec]
- Stability tests were executed on the **liquid** and the **solid** (agent: agarose) phase of **QC materials**



## STRESS TEST

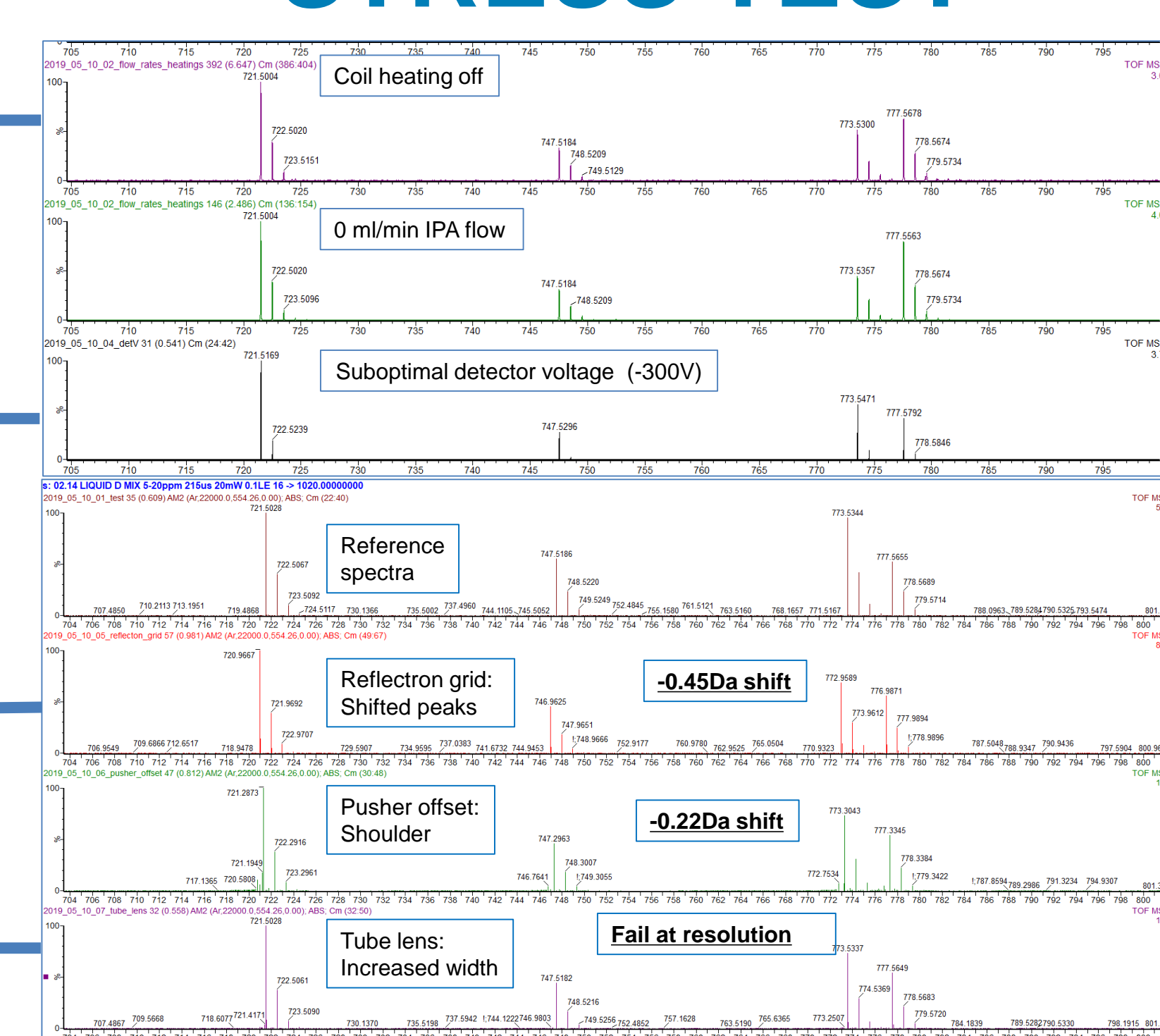


Figure 4: Spectra about the effect of the stress test (D liquid 20s scans)

- REIMS users can be provided with an applicable **Quality checking software** and material.

## AIMS

To determine the performance of the **Rapid Evaporative Ionization Mass Spectrometry (REIMS)** in terms of **long-term reproducibility**

## RESULTS LONG-TERM REPRODUCIBILITY

Thermal ablation	Sampling	2016	2017	2018	2019
iKnife probe	Manual		B. liver 1st set		
iKnife probe	Manual		B. muscle 1st set		
iKnife probe	Manual	B. liver 2nd set	B. liver 3rd set		
CO2-laser	Robotic			Bovine liver 4th set	Bovine liver 5th set
Miniaturized RF generator	Robotic				
iKnife probe	Manual	B. muscle 1st set	B. muscle 2nd set		
CO2-laser	Robotic			B. muscle 3rd set	B. muscle 4th set
Miniaturized RF generator	Robotic				
iKnife probe	Manual			Certified meat standard	
CO2 laser	Manual			75% Cocoa chocolate 1st set	75% Cocoa chocolate 2nd set
	Manual			90% Cocoa chocolate 1st set	90% Cocoa chocolate 2nd set

Table 1: Timeline of the long-term reproducibility study

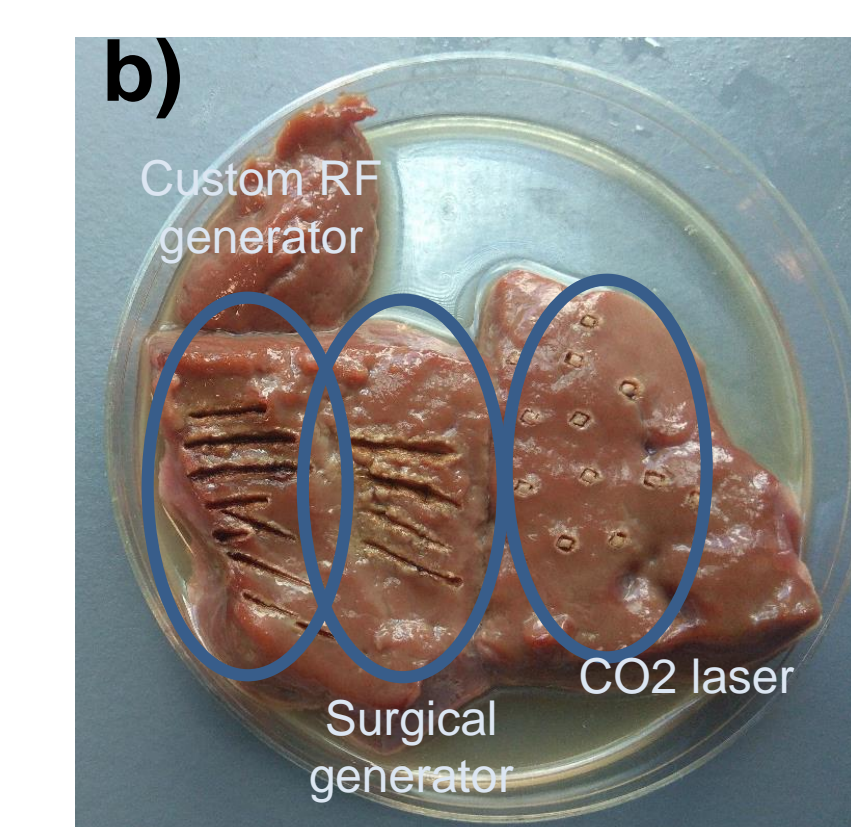
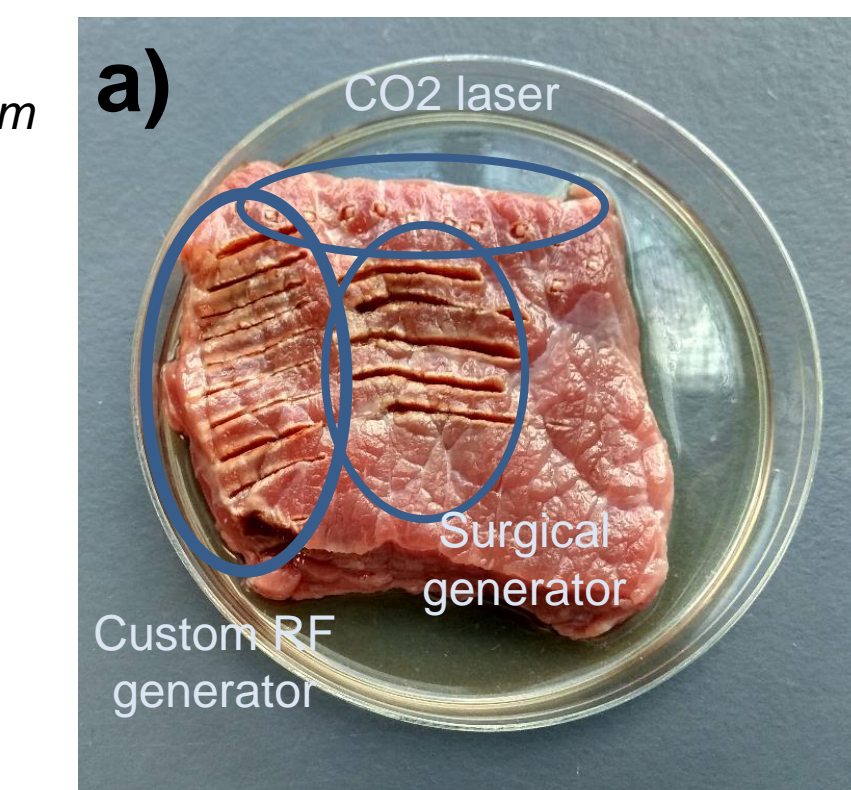


Figure 5: Different thermal ablation comparison a) bovine muscle b) bovine liver

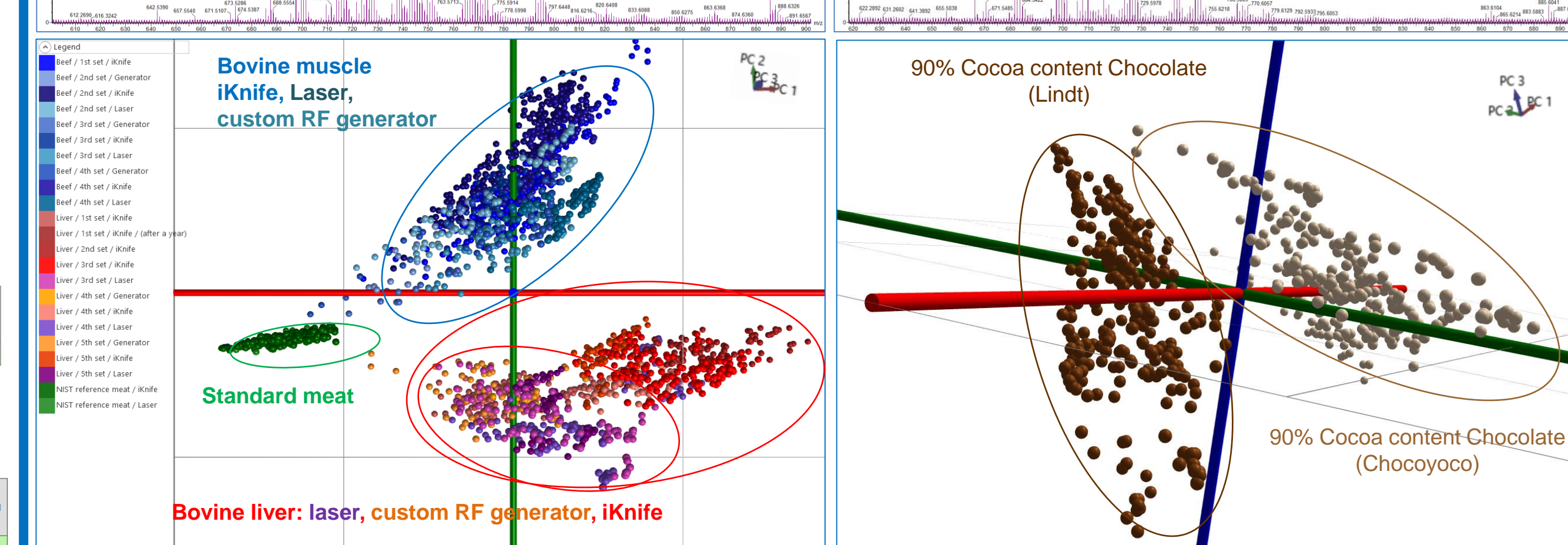
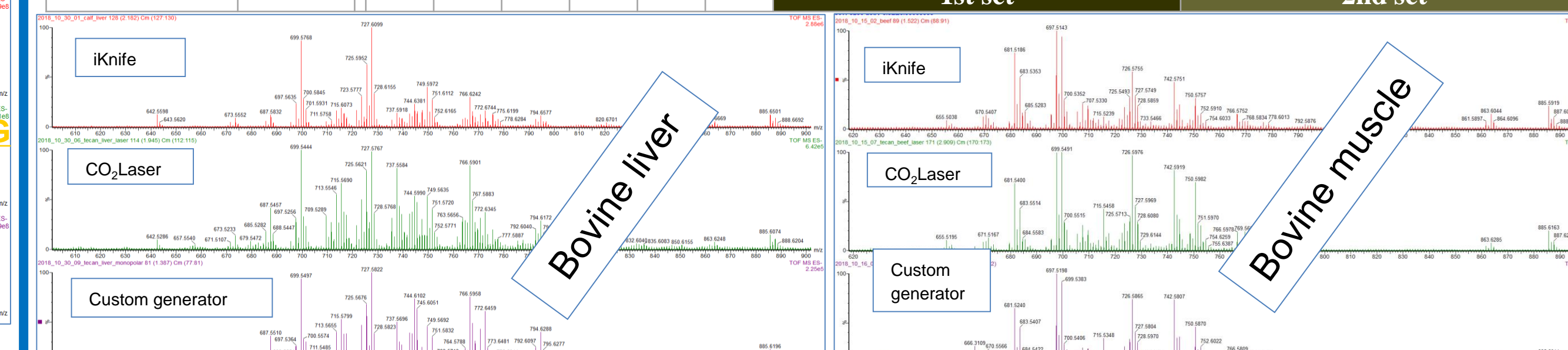


Figure 6: Spectra of the biological samples with various ablation methods [5s scans] and the PCA model of the long term reproducibility results

### Summary

Although there is variation in the data collected, classification and database building with **REIMS is stable long-term**.

	Beef	Liver	Standard meat	Outlier	Total	Classification rate	75% cocoa Chocoyoco	90% cocoa Lindt	Outlier	Total	Classification rate
Beef	1074	0	3	3	1080	99.4%	284	0	1	285	99.6%
Liver	0	982	0	46	1028	95.6%	0	278	6	284	97.7%
Standard meat	1	0	361	2	364	99.2%	0	278	6	284	97.7%
Total	1075	982	364	51	2472	97.8%	284	278	7	569	98.8%

Table 2: Confusion matrix of the long-term reproducibility study

## CONCLUSION

- It was proved that our quality control test and PG based standard is capable of making certain the REIMS system suitability.
- The pre-build database with REIMS system can be used over a long time period for characterization of liquid and solid samples