Incorporating standardised drift-tube ion mobility to enhance non-targeted assessment of the wine metabolome (LC × IM-MS)

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Outline

1) Low-field drift tube ion mobility with time-of-flight mass spectrometry (IM-TOFMS)
    Instrument design overview
    Collision Cross Section (^{DT}CCS)

2) Macedonia – an emerging wine producer
    Climate and wine growing regions
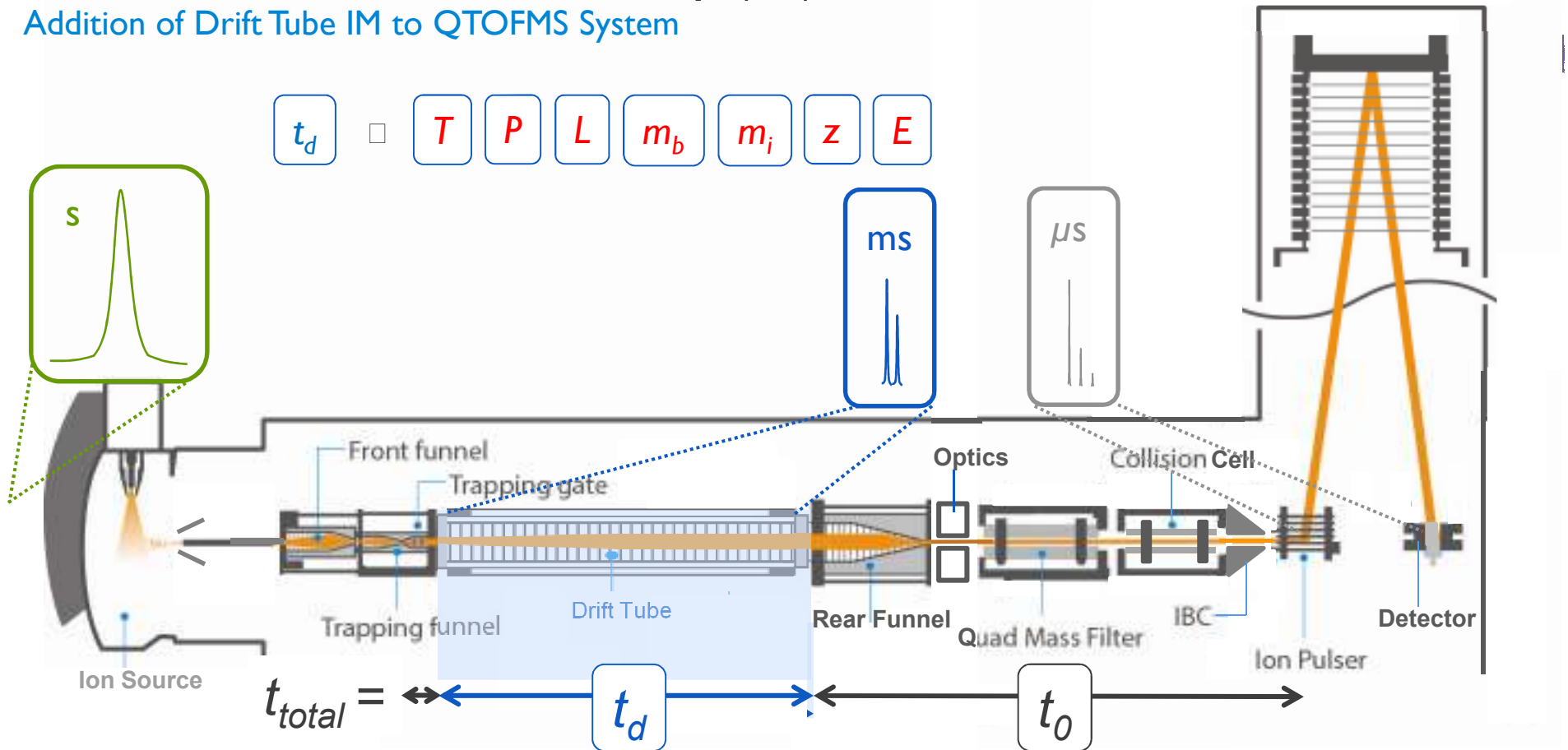   Preparation and collection of wine samples

3) Analytical workflow and results
    Wine fingerprinting
    Using ^{DT}CCS for identity confirmation

Low-field Drift Tube Ion Mobility (IM)

Addition of Drift Tube IM to QTOFMS System

t_d T P L m_b m_i z E

s

ms

μs

Front funnel
Trapping gate
Optics
Collision Cell

Drift Tube
Rear Funnel
IBC
Detector

Trapping funnel
Quad Mass Filter
Ion Pulser

Ion Source

$t_{total} = $ t_d t_0

Ion Mobility: Drift Time (t_d) and ^{DT}CCS

LC-compatible Methodology

Single-field Determination [1]:

Transient peaks allow only enough time for one field strength to be used.

Use drift times of calibrant ions (reference ^{DT}CCS values) to perform *universal linear calibration*.

Universal calibration function applied to IM-MS or LC × IM-MS files.

=> One set of calibrant ions for all metabolite classes and charge states.

[1] Fjeldsted et al, *Highly Accurate Collision Cross Section Measurements for Comprehensive High Throughput Applications,* 2016, 64th ASMS, San Antonio, USA.

Wine in Macedonia (collaboration with Štip)

Location & Climate

Republic of Macedonia

A sunny, pristine and mountainous country in the heart of the Balkans, Macedonia is a centuries-old producer of fine wines.

Mediterranean and continental climates, with warm summer days and cooler nights. Rich, heavy and clay-filled soils are good base for lengthy ripening of the grapes.

- higher concentrations of sugar, acids and phenolics
- wines with intense aroma, freshness and harmony

Wine in Macedonia

Grape varieties: red

Vranec (most economically important), Stanušina (autochthonous variety), Kratošija (Balkan variety), Pinot Noir, Merlot, Kadarka, Cabernet Sauvignon, Cabernet Franc
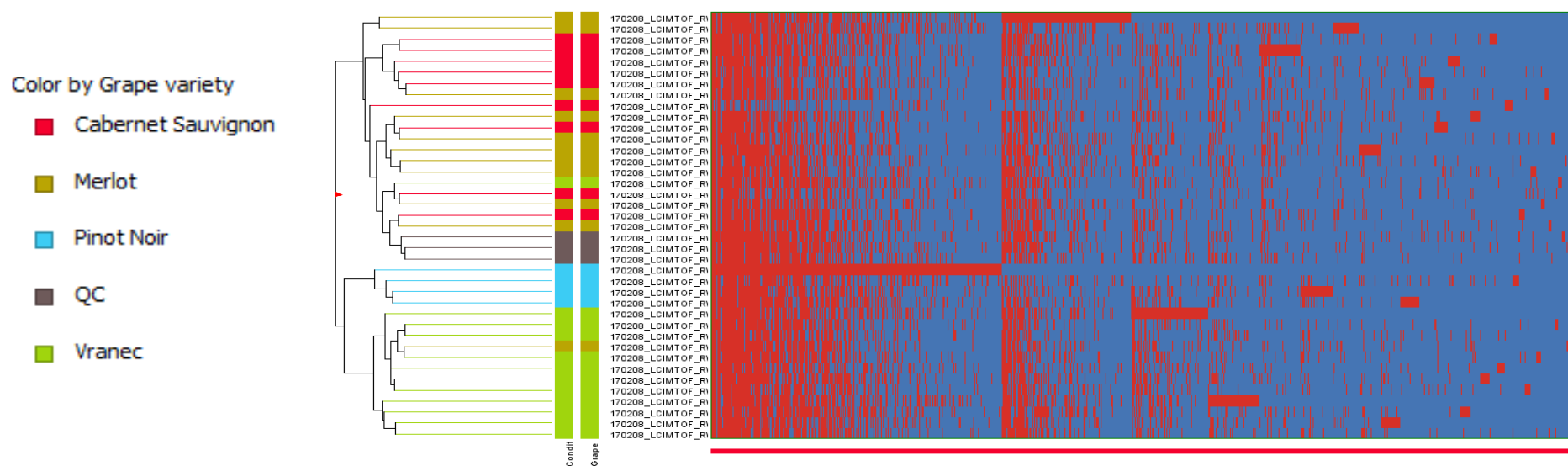

Vranec

Stanušina

Kratošija

Hierarchical Clustering on Grape Variety
Unsupervised Eucledian (Wards Linkage)

Summary
Current Status and Outlook for Metabolomics

- Wine fingerprinting is maturing, but will allow building of libraries

- Identity confirmation potential with ^{DT}CCS is powerful

- General method development for metabolomics workflows is promising, but not yet mature