Highly sensitive volatile compound fingerprinting of innovative food-related products with ion mobility spectrometry

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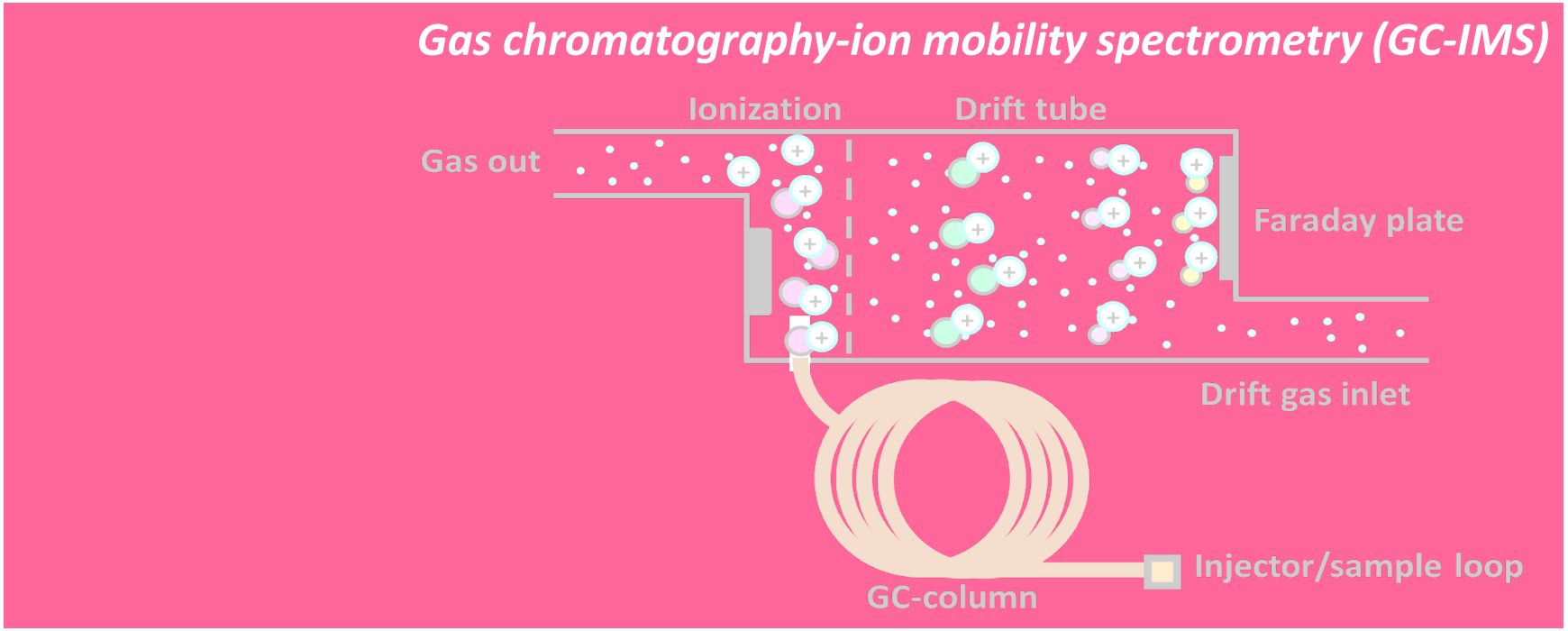
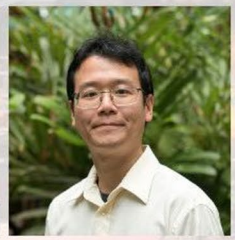


Metabolomics for Life Sciences Research Unit
Chulalongkorn University

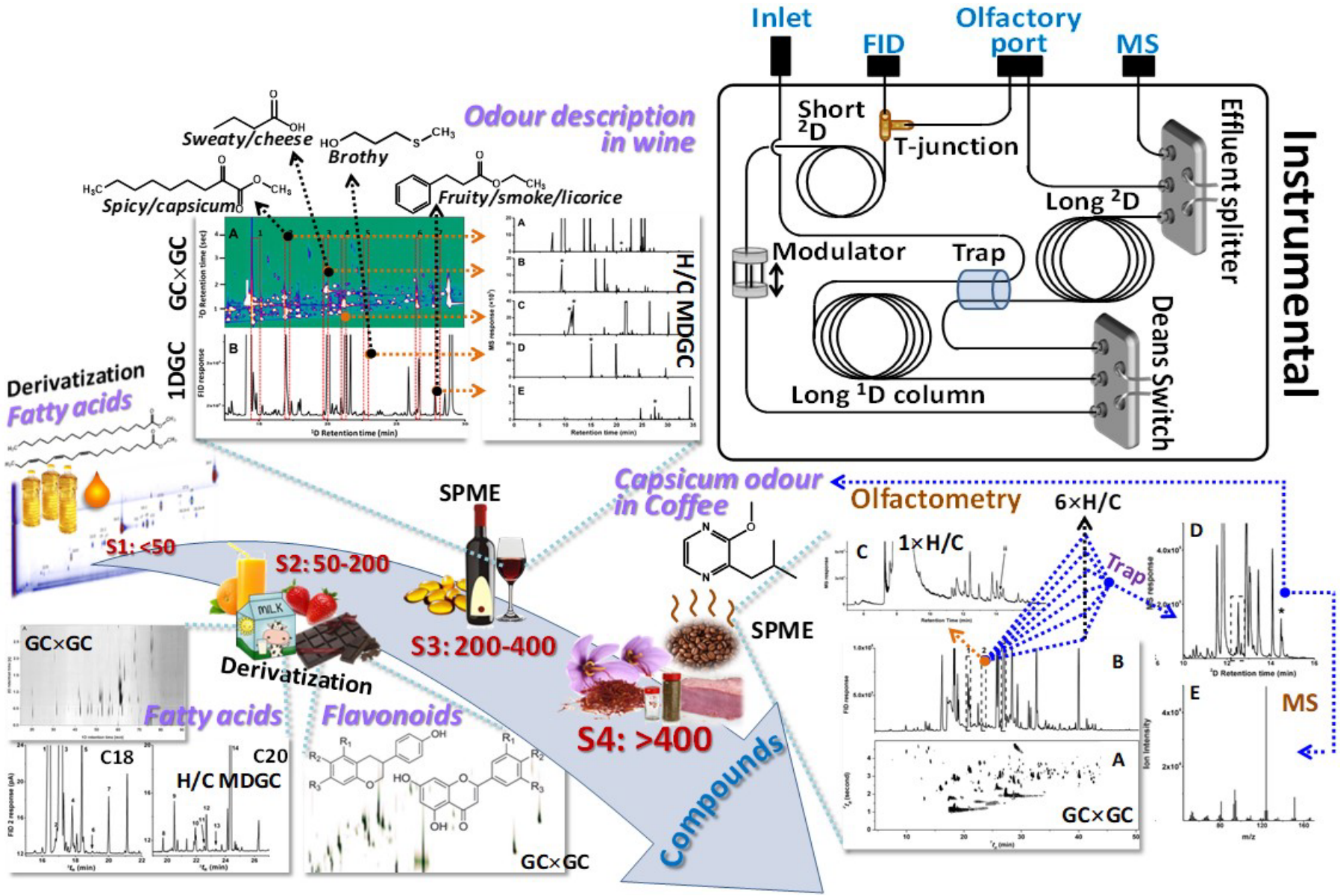






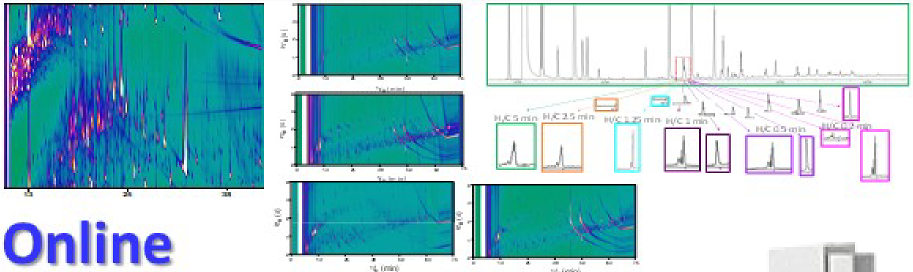

Chromato Kit Ta Nie Land
Multidimensional
Inlet
FID
Olfactory port
MS
Sample preparation
Petroleum
Herbs and plants
Odour description in wine
Capsicum odour in Coffee
50-200
200-400
>400
Triglycerides
Compounds
Food
New materials
Theoretical
Environmental
Fresher
Fluorescent
Softer & longer lasting
Adjustable smell by pressing buttons
Perfume
Office
Time (min)

Complexity of food samples & approaches in Gas Chromatography



Y. Nolvachai, C. Kulsing, P.J. Marriott, *Trends in Analytical Chemistry*, 96 (2017) 124-137

Approaches for volatile fingerprinting analysis



Online

Chromatographic approach

Conventional two-dimensional GC (GC×GC)

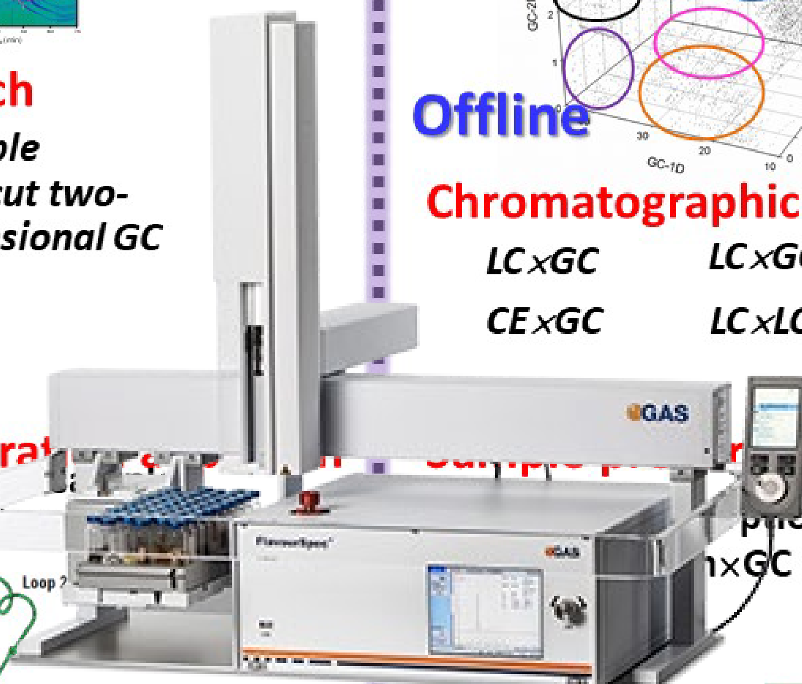
Multiple heartcut two-dimensional GC

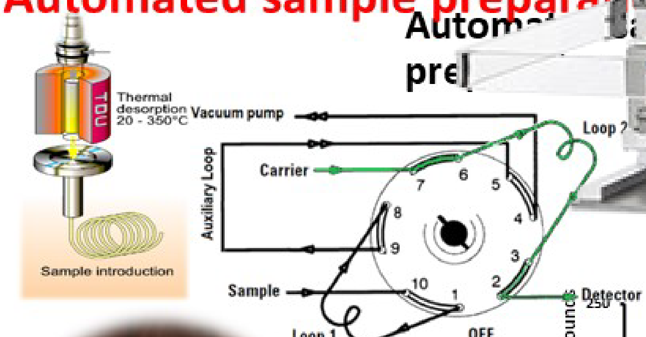
GC–Comprehensive MS/MS

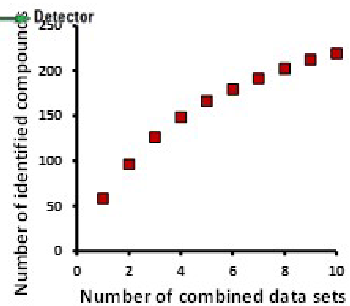
Automated sample preparat

Autom

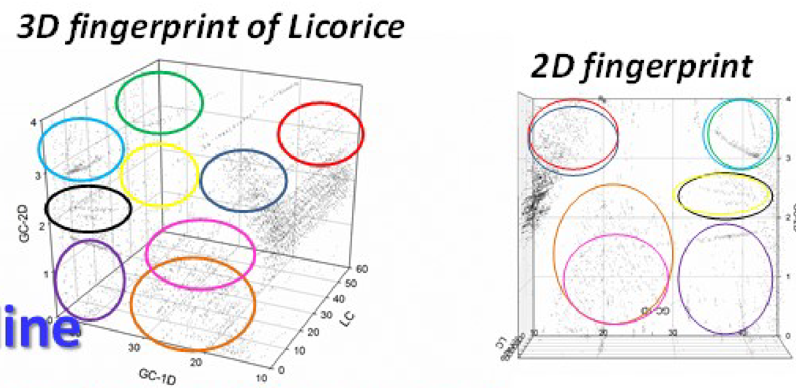
pre







Offline



Chromatographic approach

LC×GC

LC×GC×GC

CE×GC

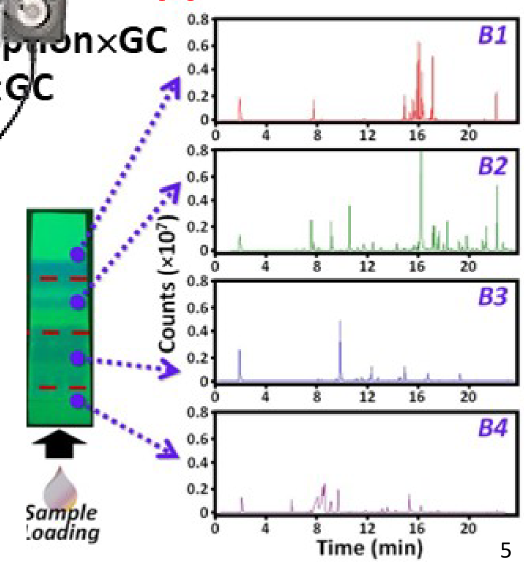
LC×LC×GC

on approach

n×GC

n×GC

•2DTLC×GC



Gas chromatography ion-mobility spectrometry (GC-IMS)

GC-IMS

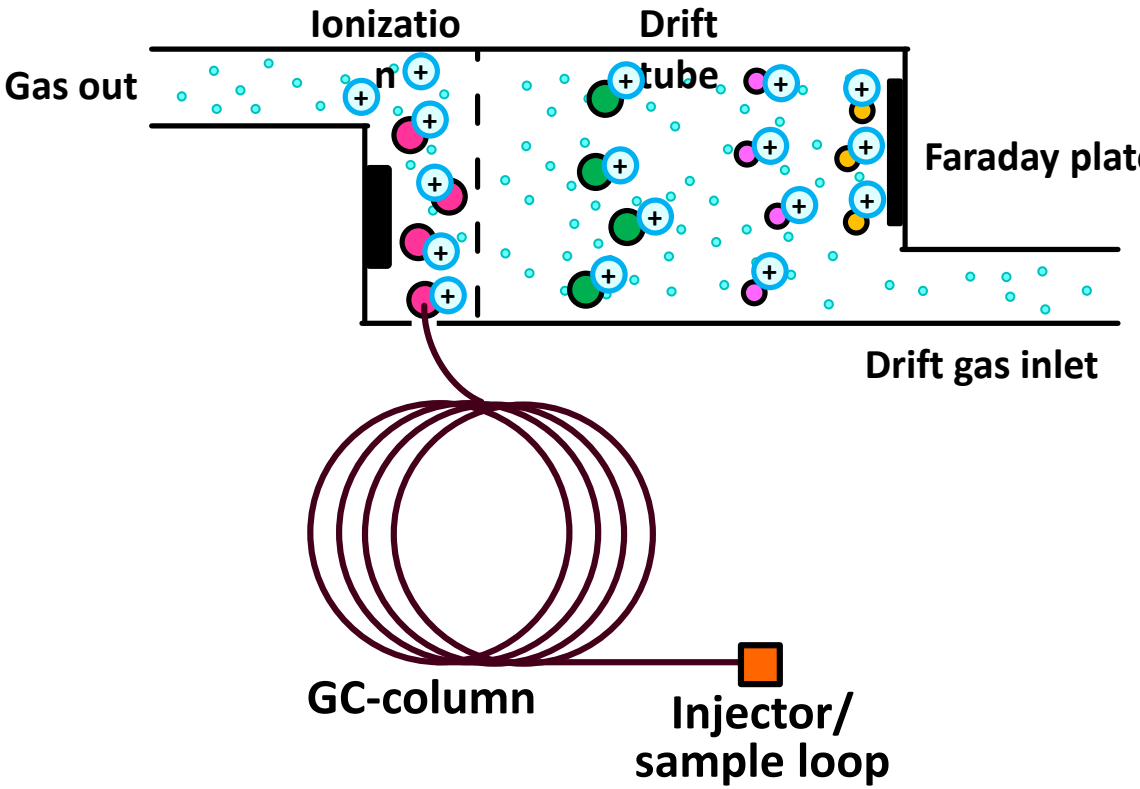
- Ion-Mobility Spectrometry
- Direct headspace/liquid injection
- Peak identification based on standard injection
- Ultrahigh sensitivity
- Highly volatile compound separation

GC-MS

- Mass Spectrometry
- Sample preparation and injection
- Peak identification based on library match
- Limited sensitivity
- Highly volatile compound coelution

Gas chromatography ion-mobility spectrometry (GC-IMS)

Injector → Column → Detector (IMS) → Ionization → IMS Drift Tube → Faraday plate



$$K = \frac{3}{16}\sqrt{\frac{2\pi}{\mu k_B T}}\frac{ze}{N\Omega}$$

K = The ion mobility

Ω = The collision cross section

T = Gas Temperature

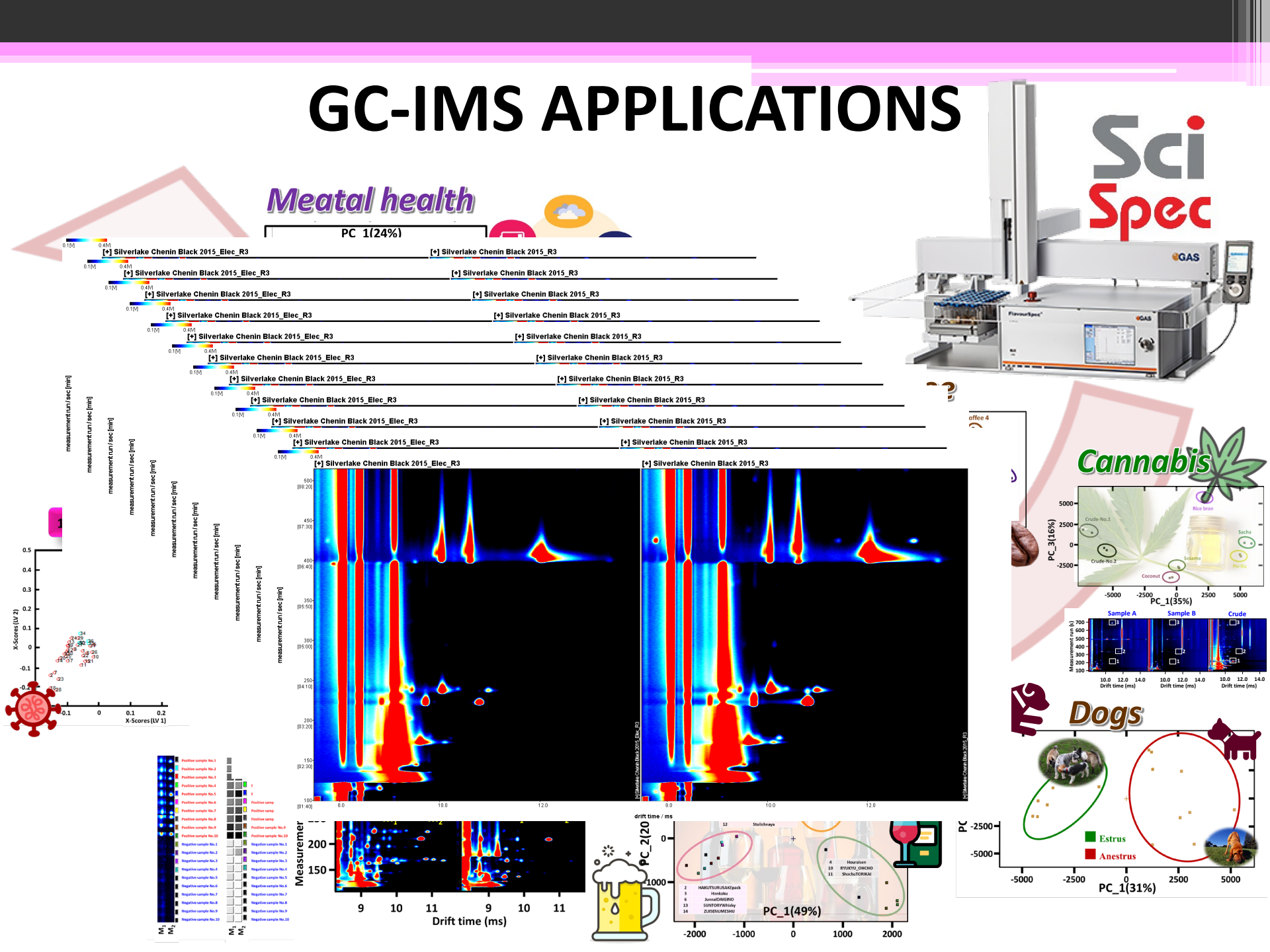
N = The gas number density

k_B = The Boltzmann constant

Ze = The analyte charge

μ = The reduced mass of the ion-gas pair

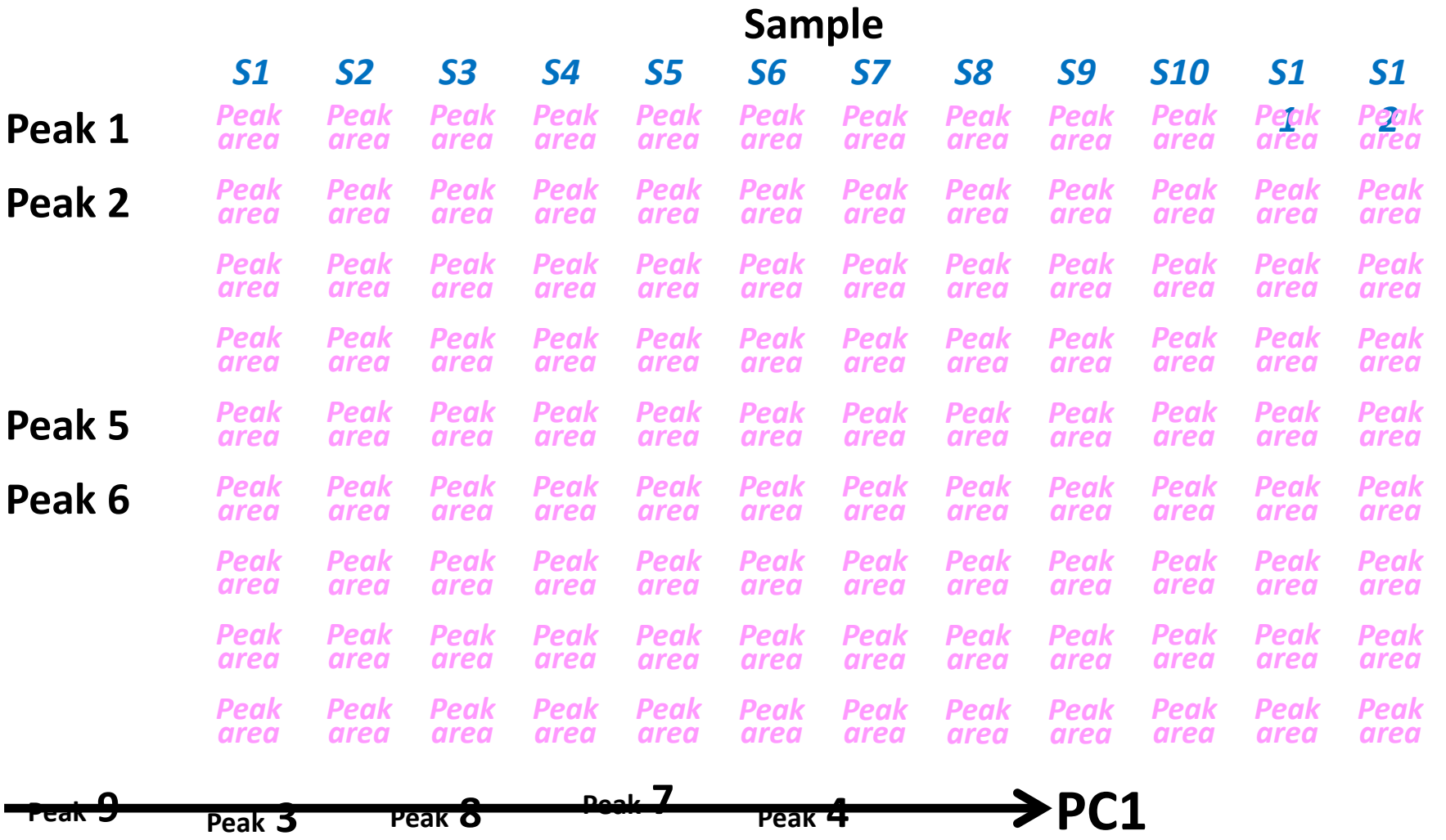
GC-IMS APPLICATIONS



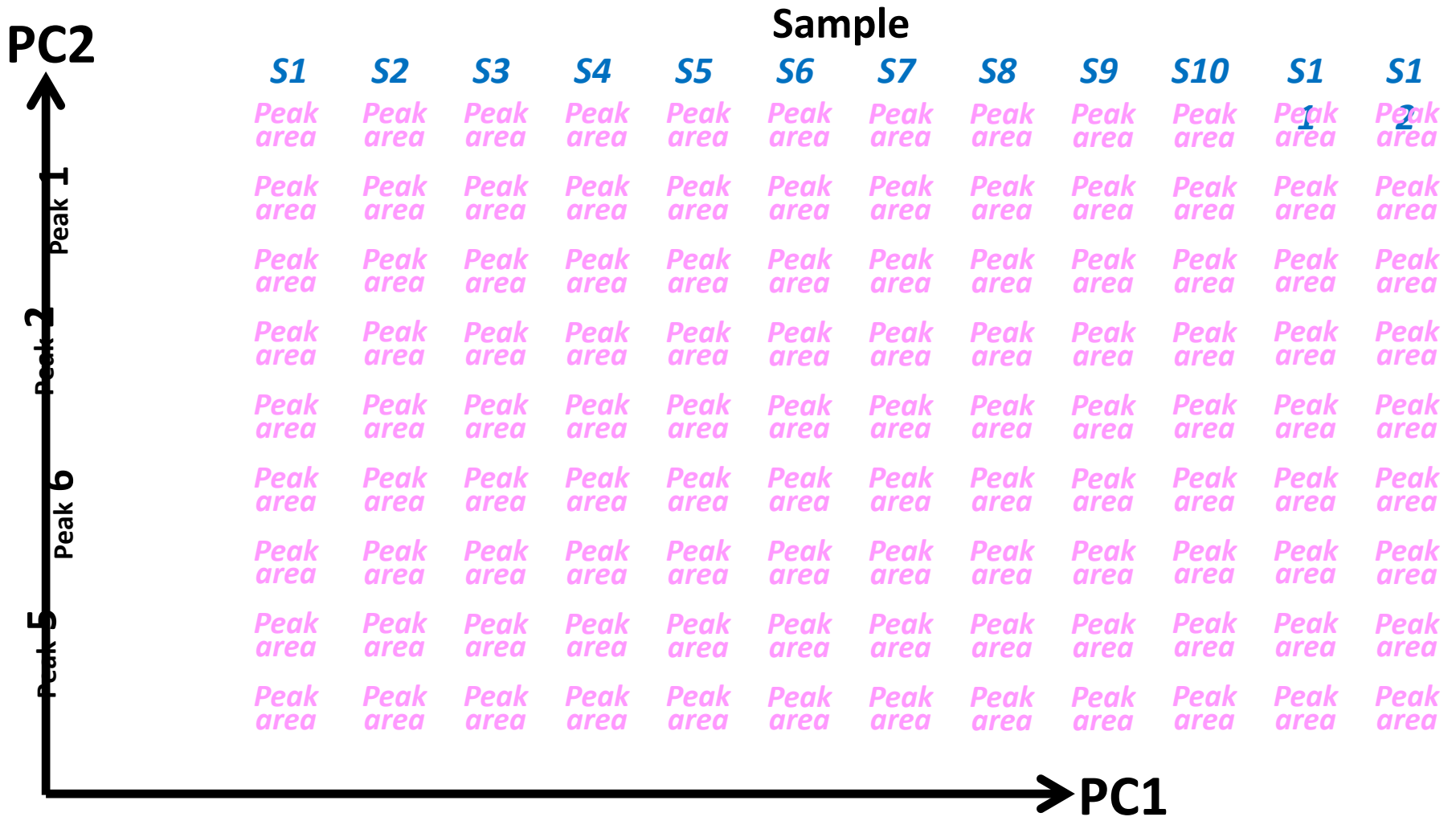
Data alignment

	Sample											
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S1 1	S1 2
Peak 1	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area
Peak 2	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area
Peak 3	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area
Peak 4	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area
Peak 5	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area
Peak 6	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area
Peak 7	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area
Peak 8	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area
Peak 9	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area	Peak area

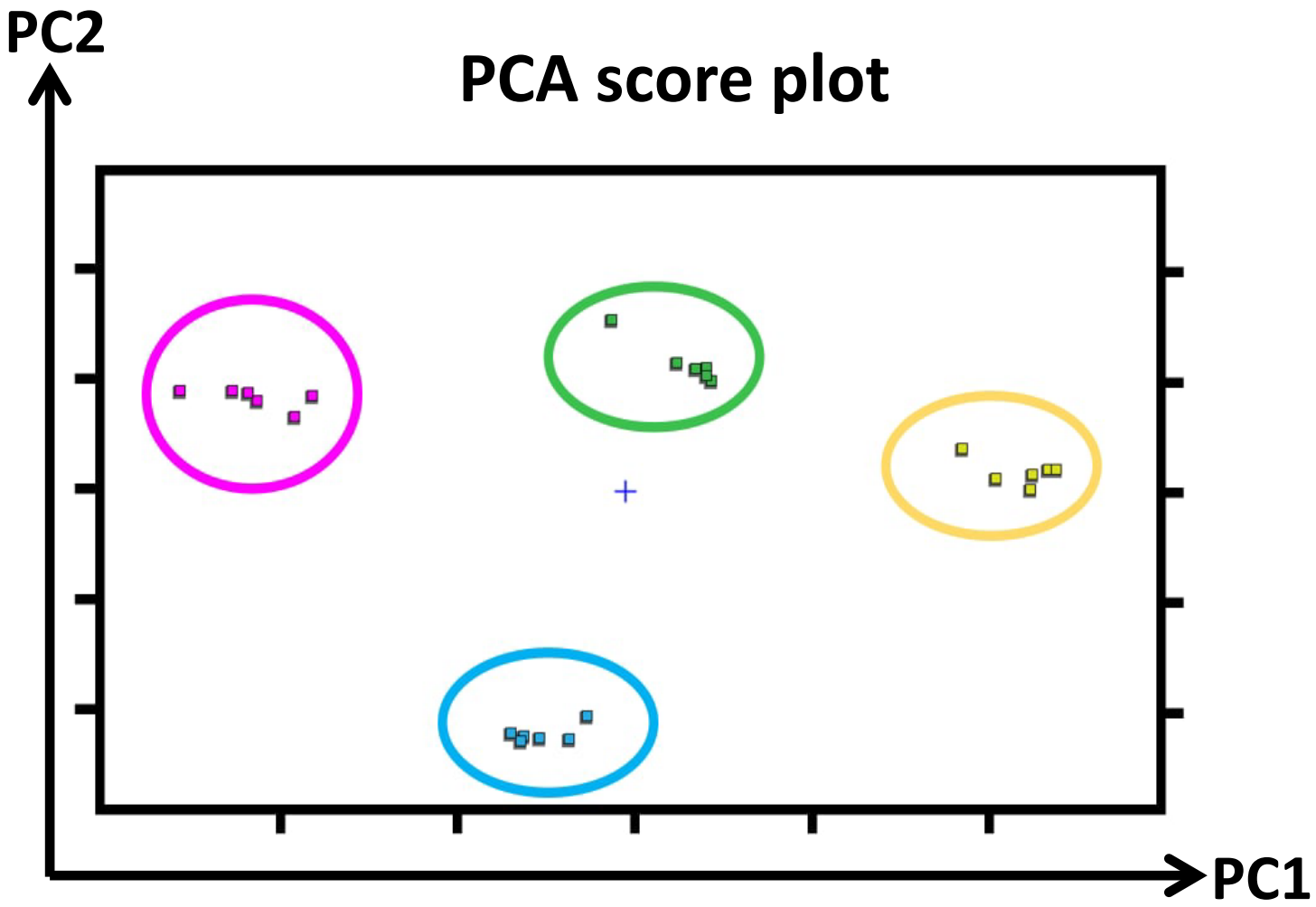
Principal component analysis (PCA)



Principal component analysis (PCA)

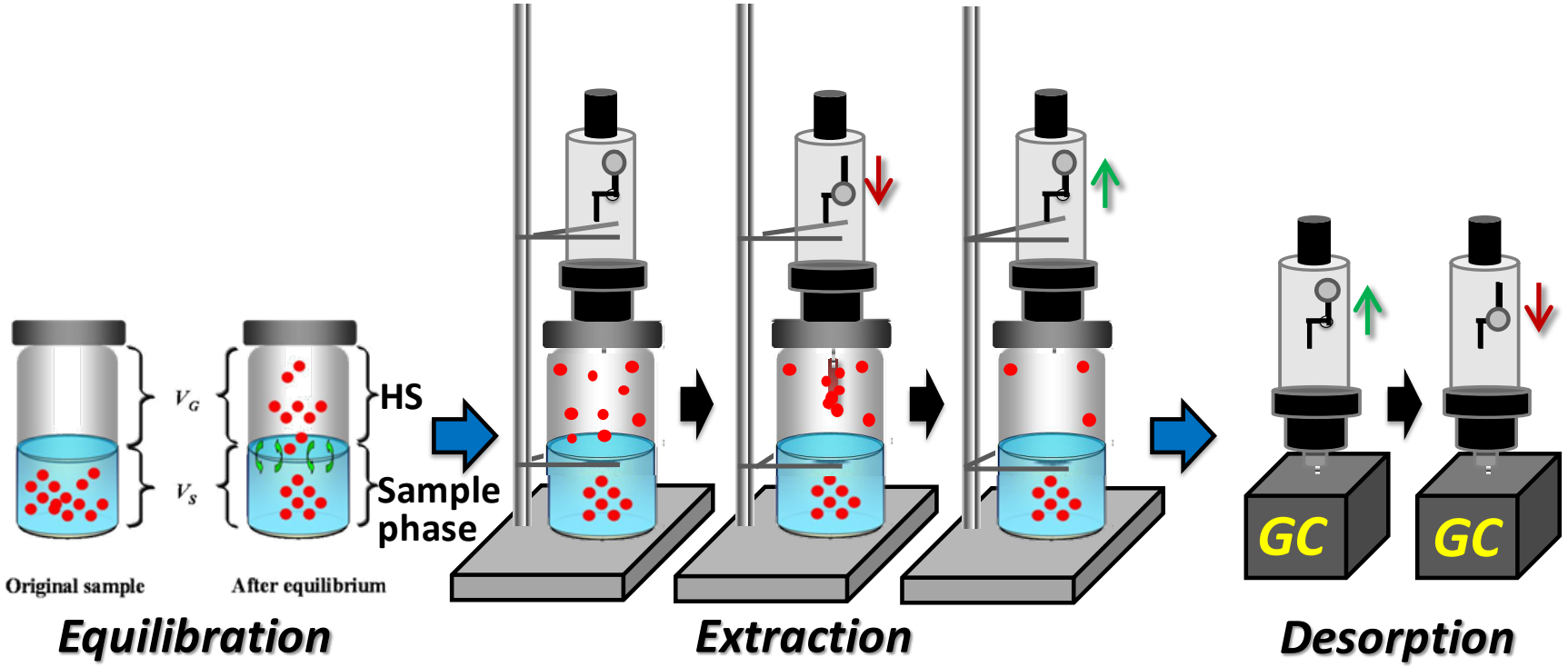


Principal component analysis (PCA)

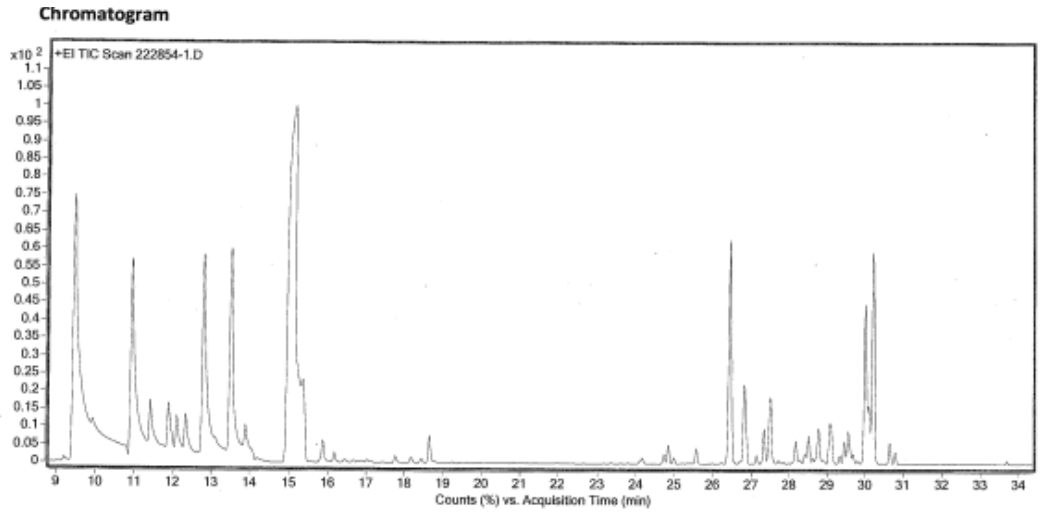


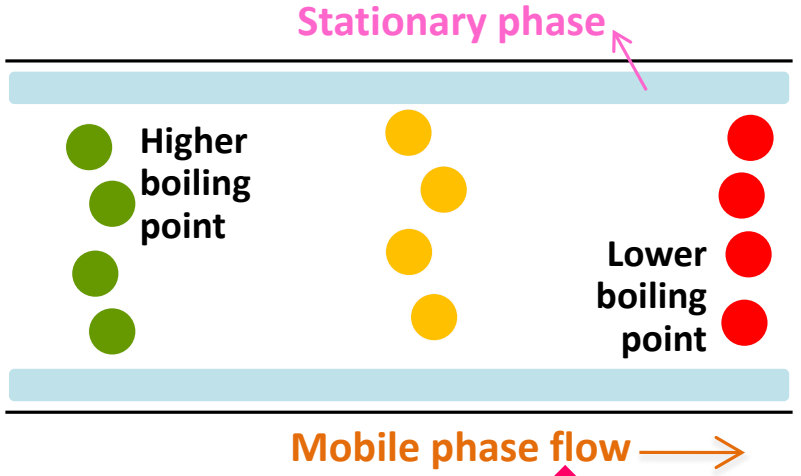
GC-IMS analysis of volatile organic compounds in cannabis samples

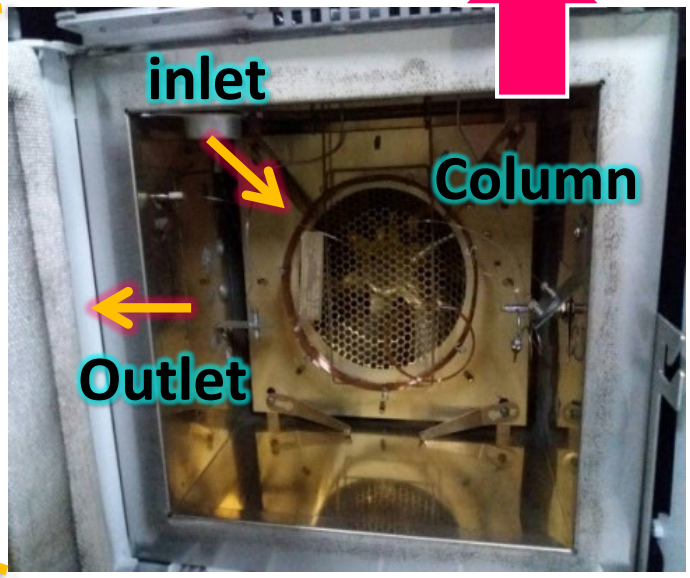
Untargeted analysis with SPME GC-MS



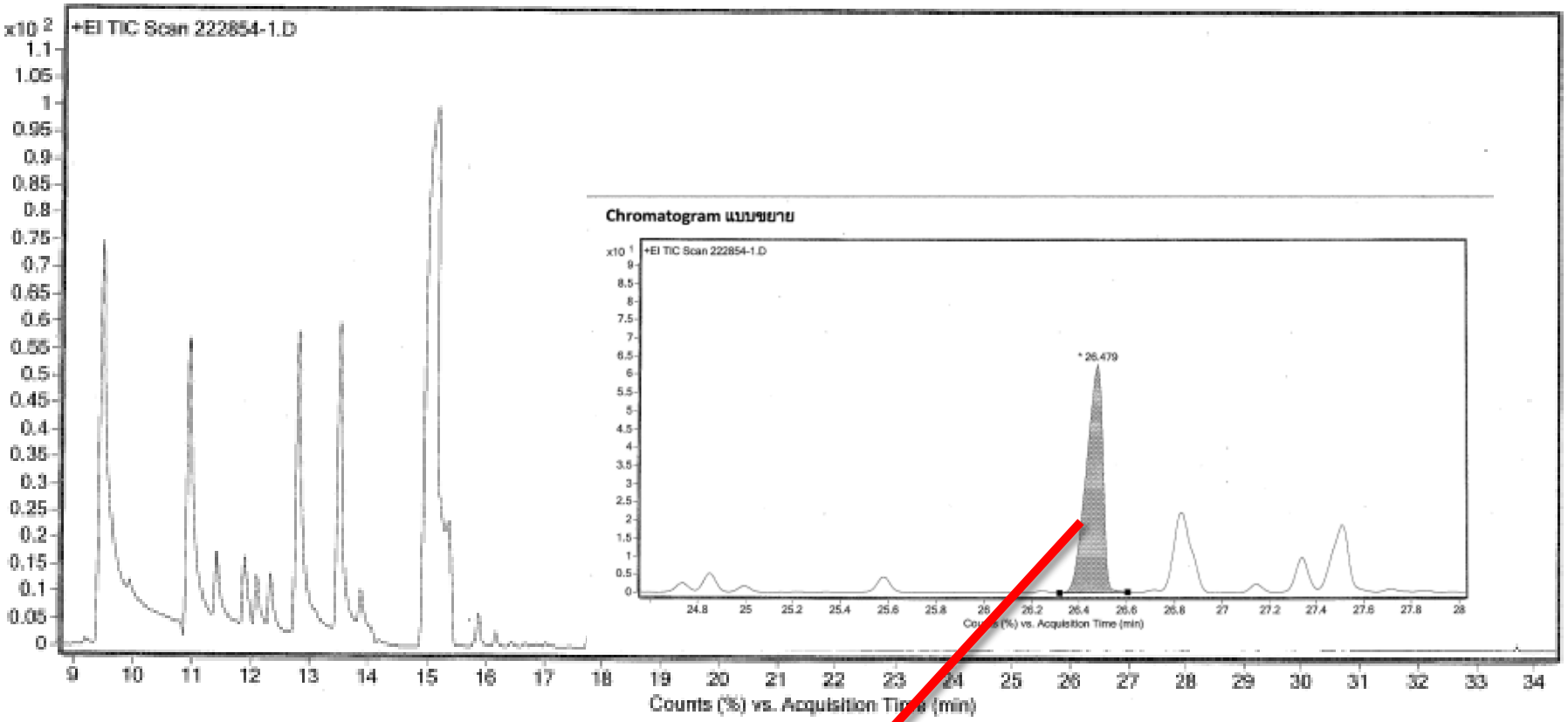
Untargeted analysis with SPME GC-MS





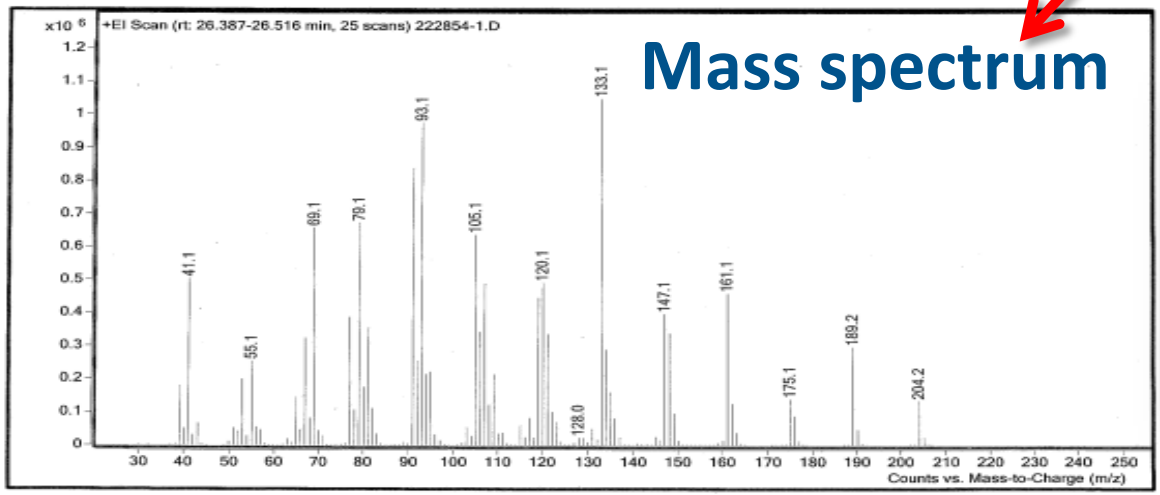


Chromatogram

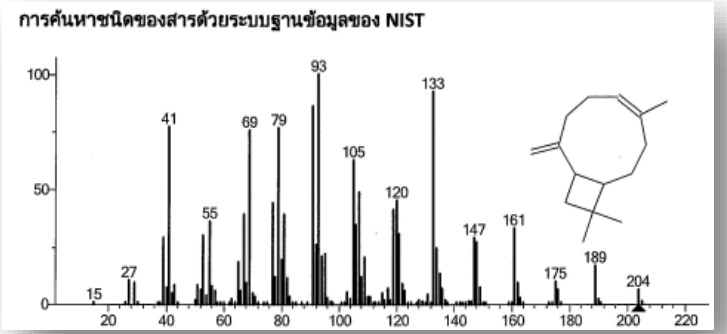


Chromatogram แบบขยาย

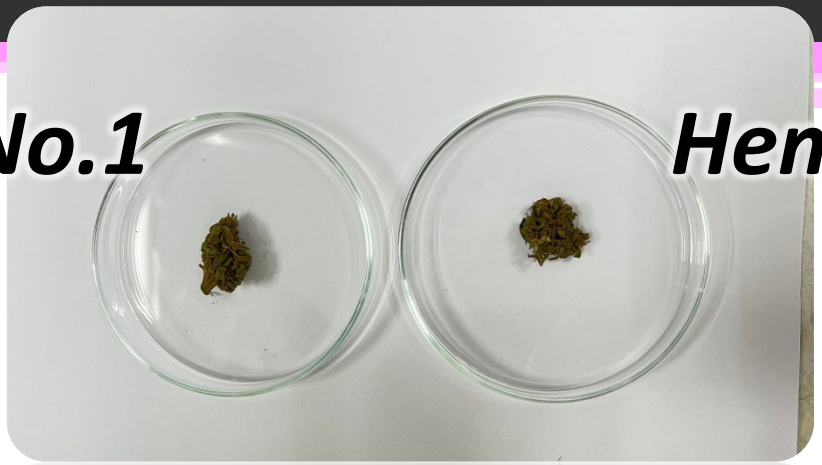
Mass spectrum



การค้นหาชนิดของสารด้วยระบบฐานข้อมูลของ NIST

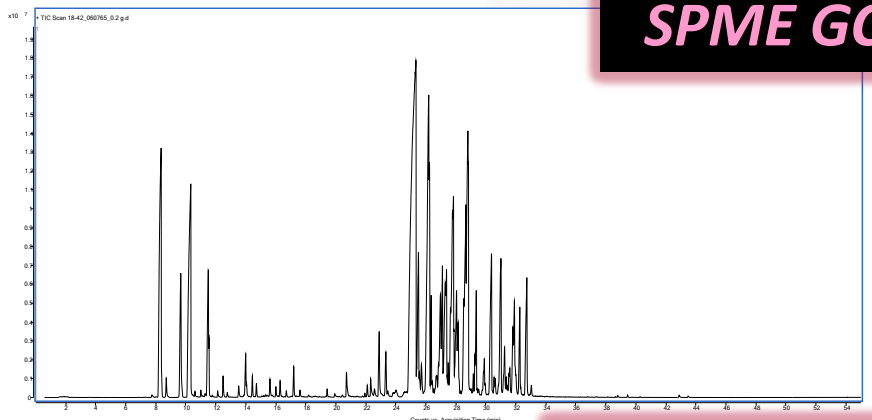


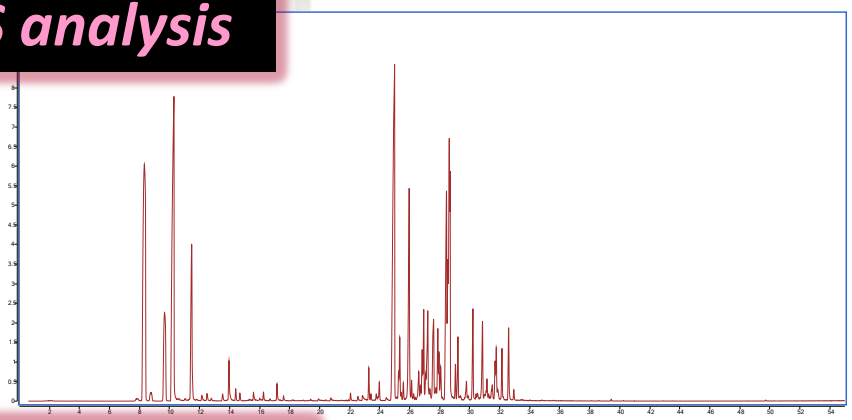
Hemp No.1



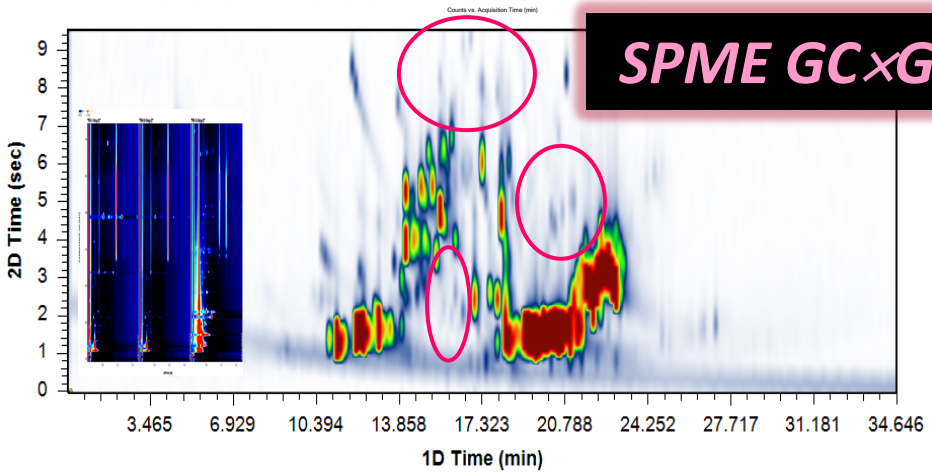
Hemp No.2

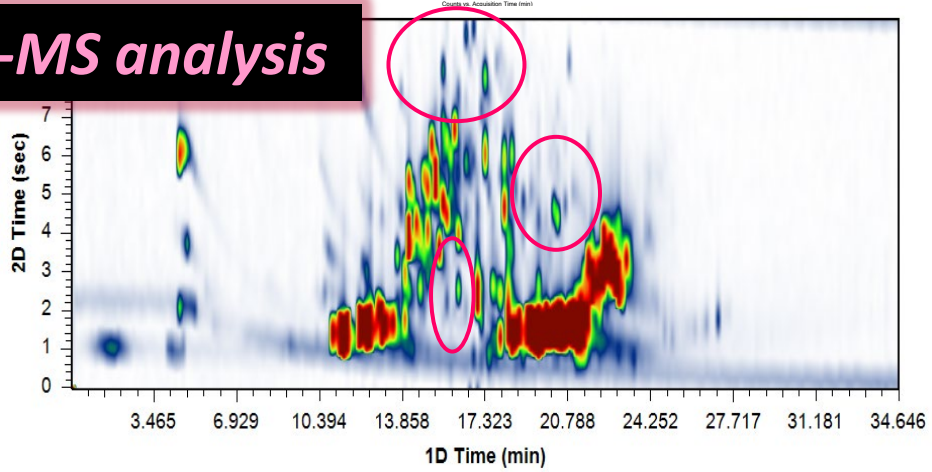
SPME GC-MS analysis



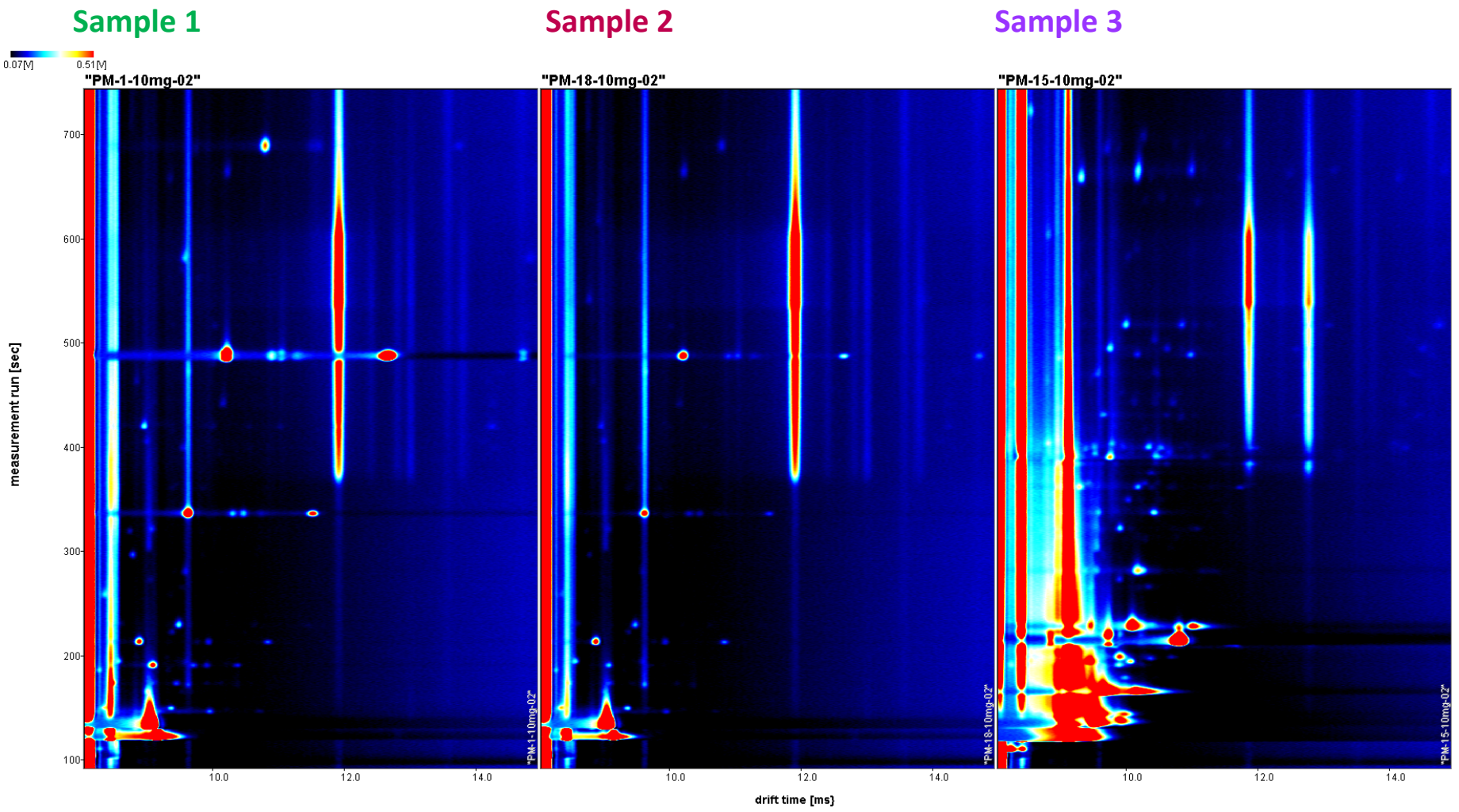


SPME GC×GC-MS analysis

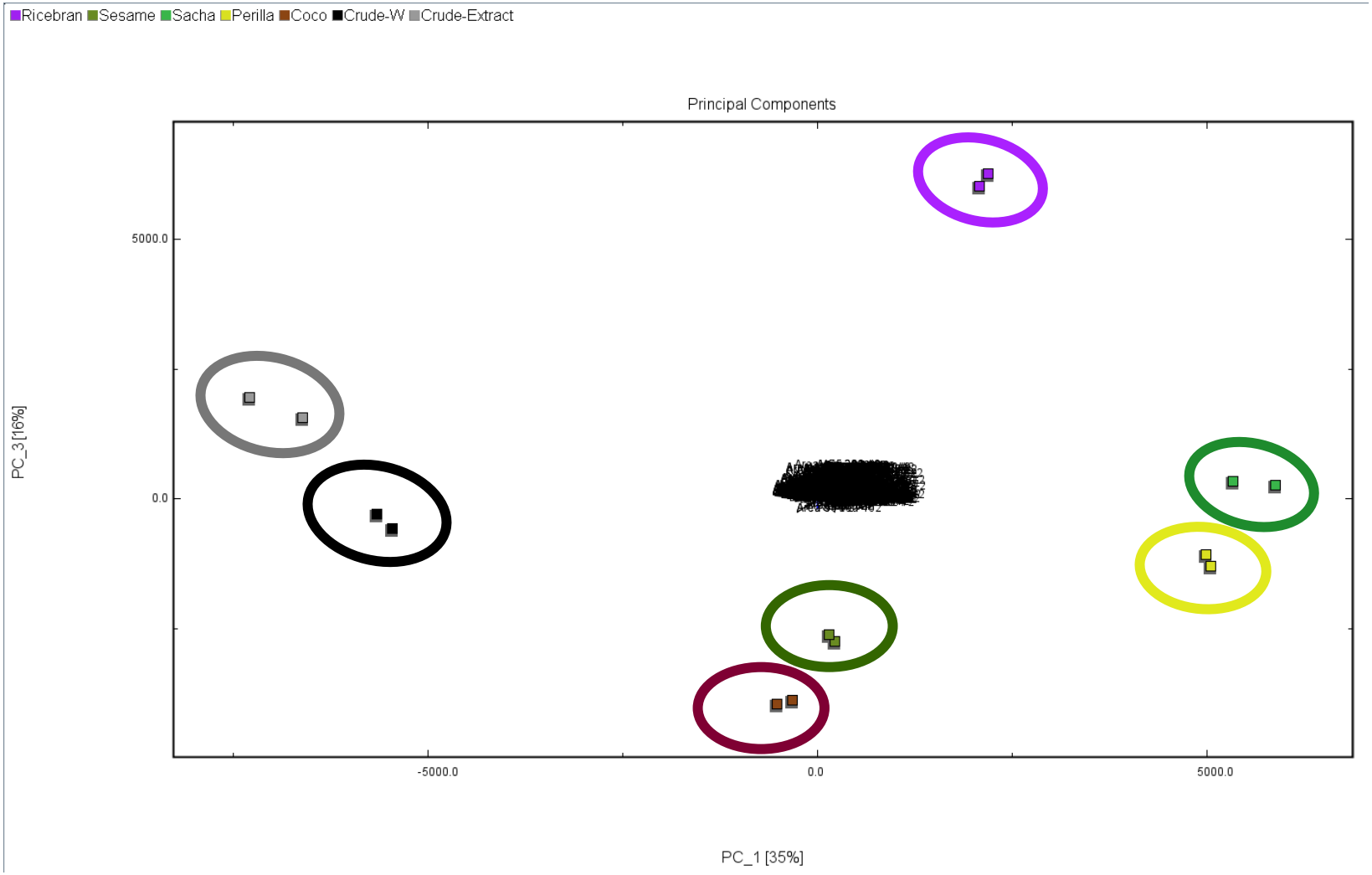




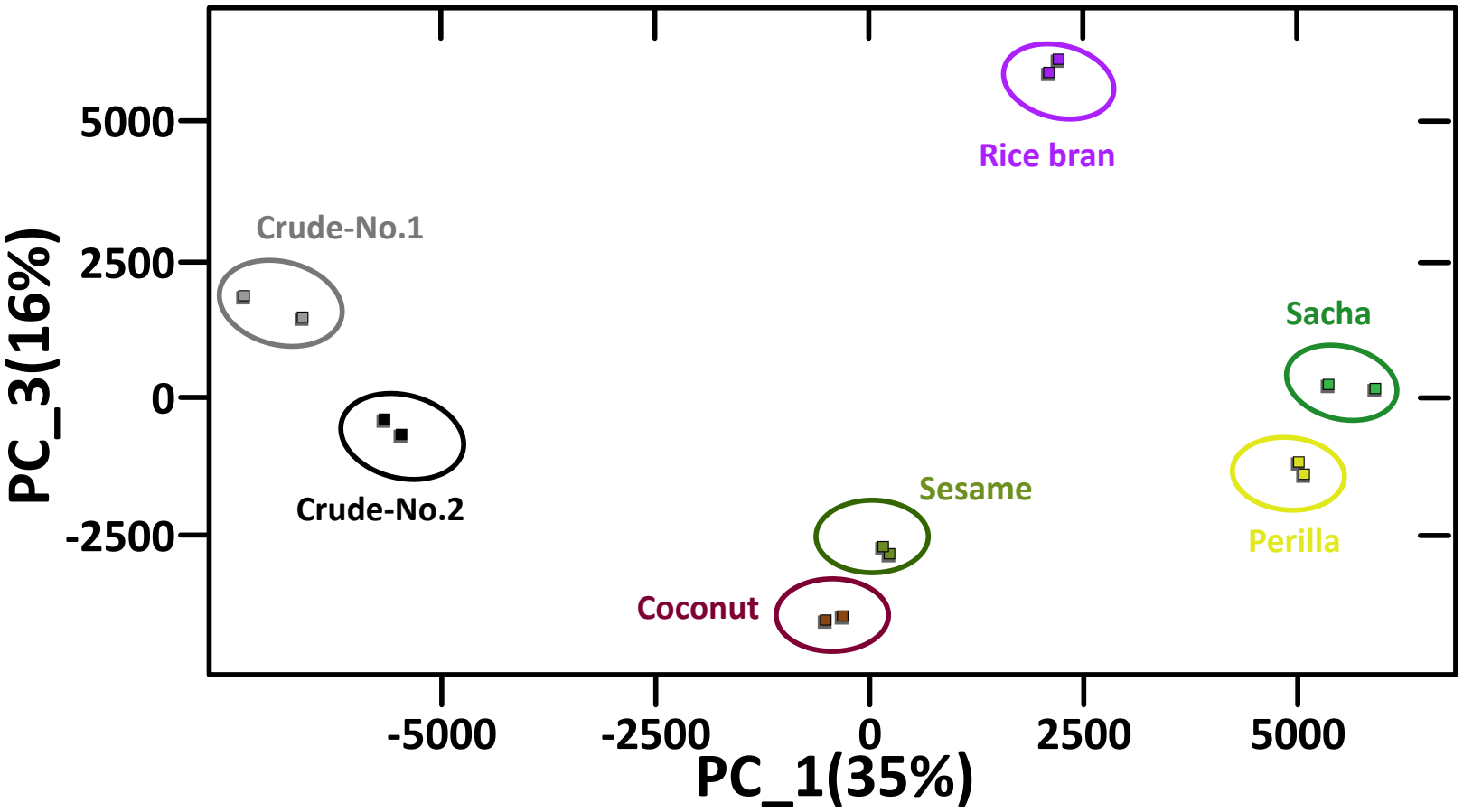
GC-IMS analysis of cannabis extracts obtained from different sources



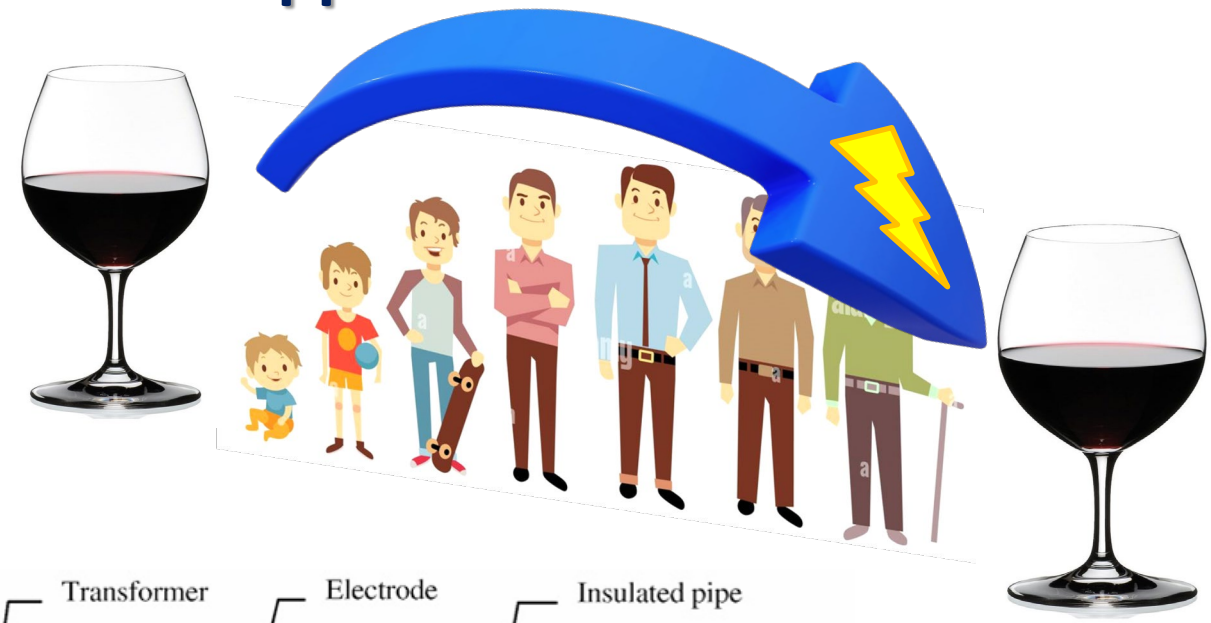
GC-IMS analysis of cannabis extracts obtained from different sources



Cannabis samples



Innovative wine maturation approach



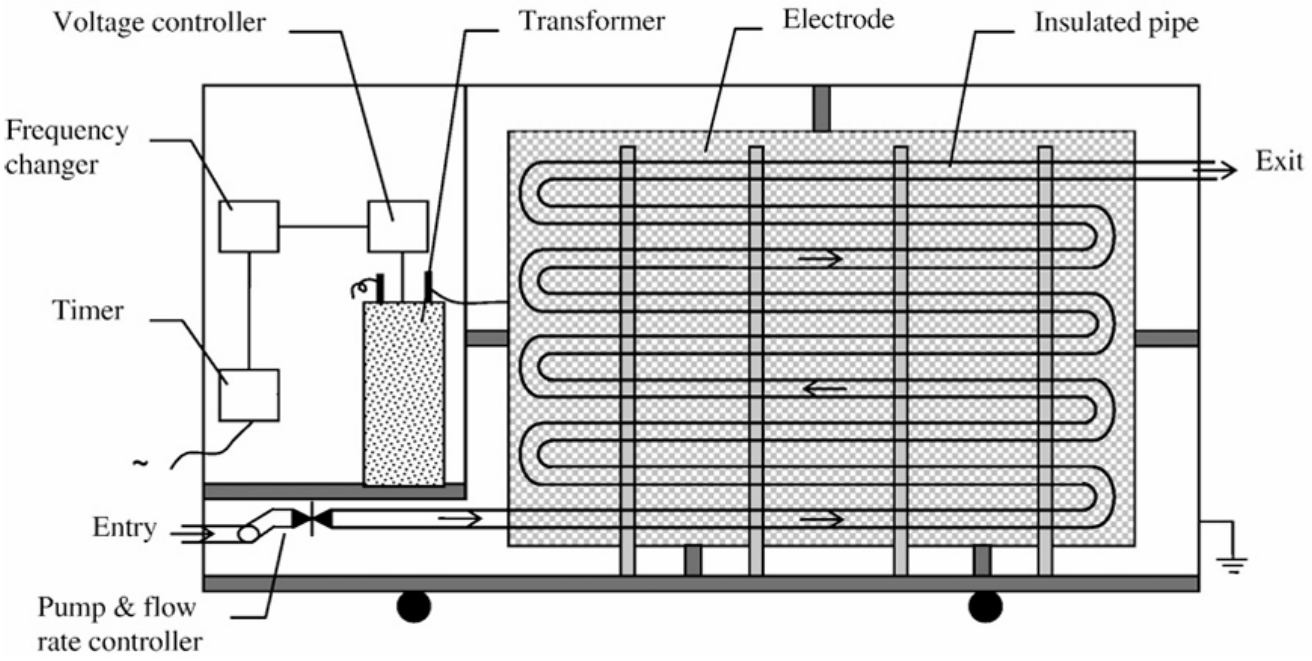


Fig. 1. Configuration of the pilot plant scale electric field set up for wine aging.

Innovative Food Science and Emerging Technologies 9 (2008) 463–468.

Innovative wine maturation approach

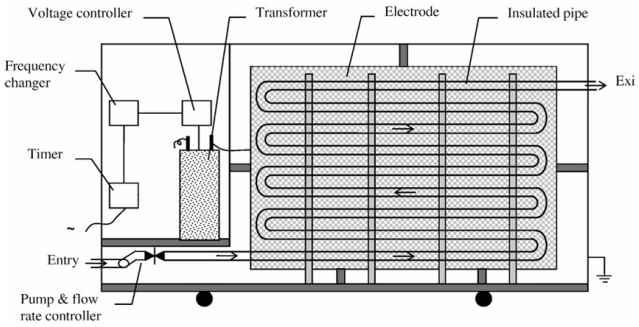


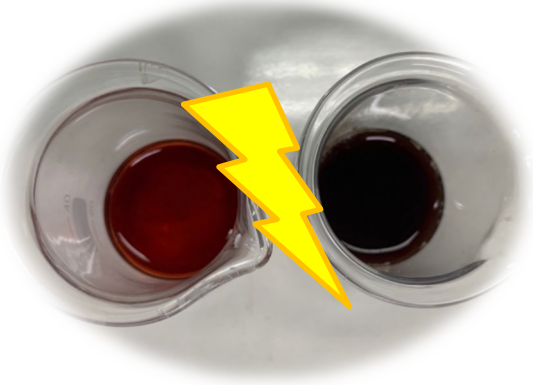
Fig. 1. Configuration of the pilot plant scale electric field set up for wine aging.

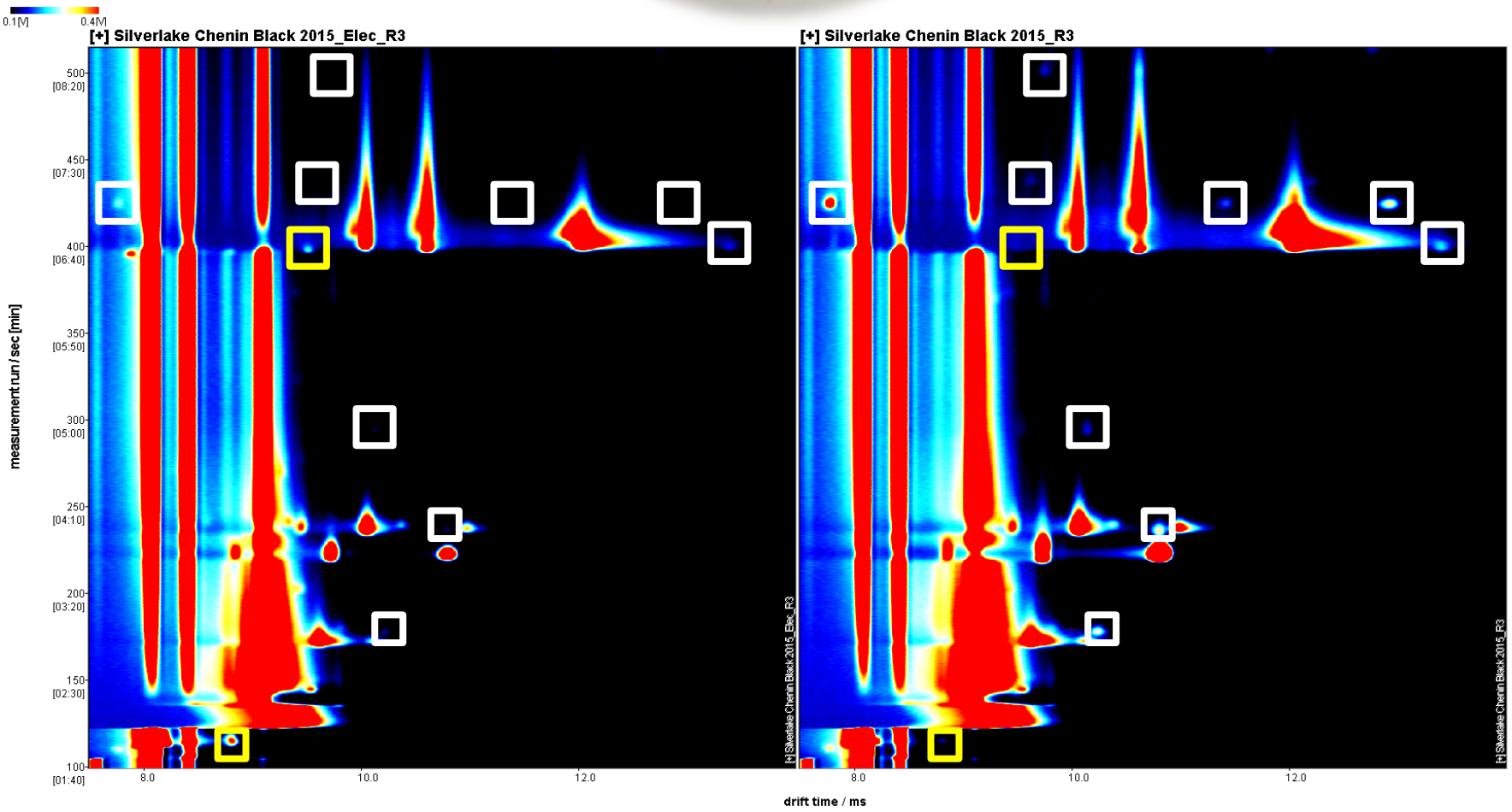
Table 2
Sensory evaluation of AC electric field treated wines with different treatments contrast to the untreated one

Samples	Electric field (v/cm)	Treat time (min)	Sensory evaluation (Scores)					Total scores (total 100)	Comments
			Clarity (total 10)	Color (total 10)	Aroma (total 30)	Taste (total 40)	Typicality (total 10)		
0	0	0	8.0	7.5	20.0	28.0	7.0	70.5	Clear, ruby red color, pungent alcohol scent with intense fruit aroma, full-bodied while astringent, unbalanced harsh taste
1-1	300	1	8.0	7.5	20.5	30.0	7.0	73.0	Astringency decreased slightly, others unchanged
1-2	300	3	8.0	7.5	22.0	32.5	7.0	77.0	Smell and taste trended to soft and harmony, others unchanged
1-3	300	8	8.0	7.5	22.5	33.5	7.5	79.0	Aged wine scent appeared, the balance of taste improved
2-1	600	1	8.0	7.5	22.0	33.5	7.5	78.5	Slight aged wine aroma, complexity improved and balanced
2-2	600	3	8.0	8.0	25.5	35.0	8.5	85.0	Pleasing fruit and aged wine fragrance, full-bodied while well-balanced and harmonious taste with perfect typicality
2-3	600	8	8.0	8.0	23.5	34.5	8.0	82.0	New unpleasant scent and coarse taste emerged
3-1	900	1	8.0	7.5	22.0	34.0	7.5	79.0	Fresh fruit smell faded while aged wine scent emerged. Softer mouthfeel while unbalanced taste acquired.
3-2	900	3	8.0	8.0	19.5	31.5	6.5	73.5	Faint new unpleasant scent blended with aged wine aroma, complexity improved while unbalanced
3-3	900	8	8.0	8.0	17.5	28.5	6.5	68.5	Burning, disharmonious mouthfeel with unpleasant scent, unacceptable change

Innovative Food Science and Emerging Technologies 9 (2008) 463–468.


CASTLE CREEK




0.1[V]
0.4[V]
[+] Silverlake Chenin Black 2015_Elec_R3
[+] Silverlake Chenin Black 2015_R3
measurement run / sec [min]
500 [08:20]
450 [07:30]
400 [06:40]
350 [05:50]
300 [05:00]
250 [04:10]
200 [03:20]
150 [02:30]
100 [01:40]
8.0
10.0
12.0
drift time / ms
[+] Silverlake Chenin Black 2015_Elec_R3
[+] Silverlake Chenin Black 2015_R3

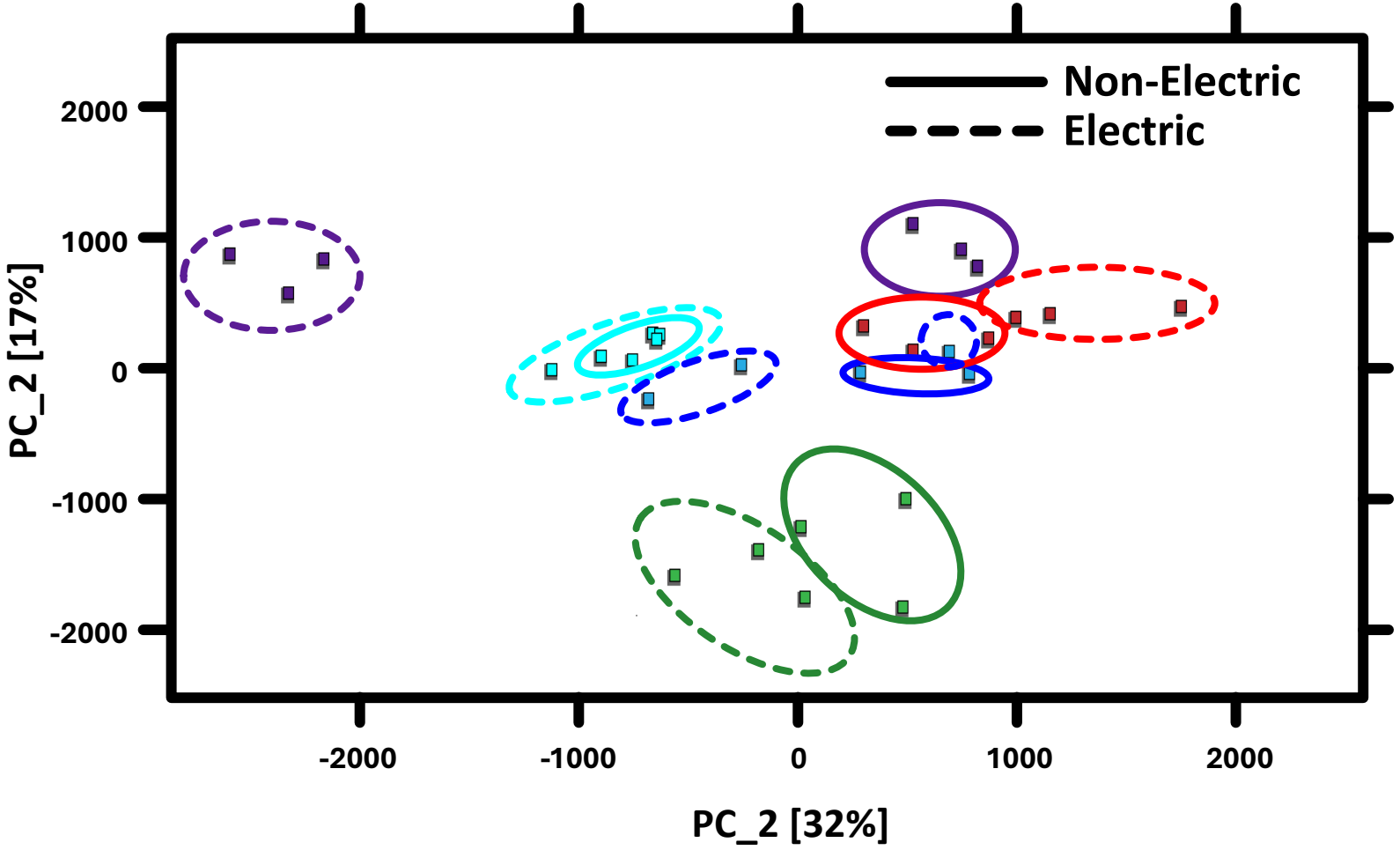
Silverlake Shiraz 2014

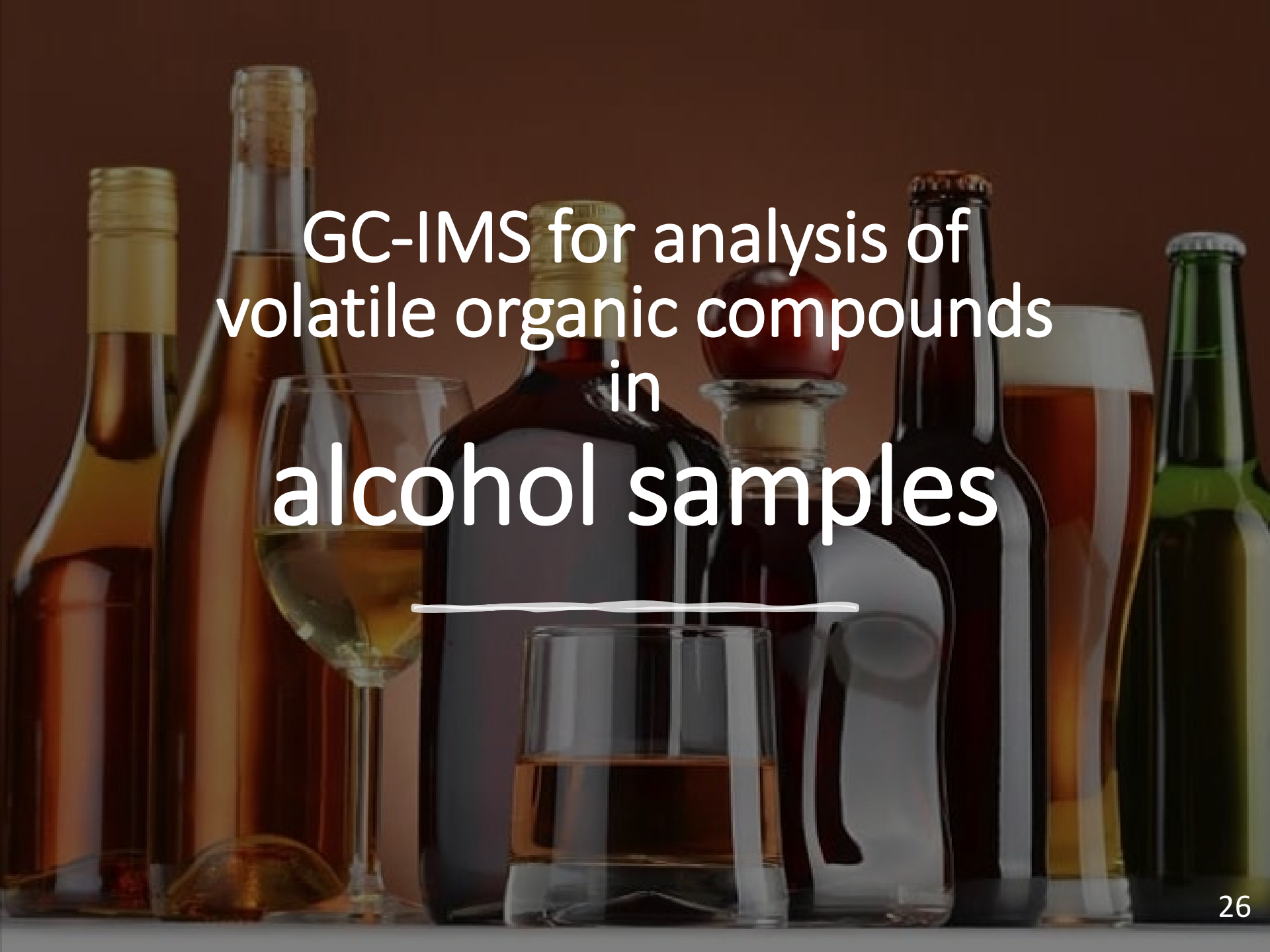
Fat Bastard Syrah 2016

Silverlake Chenin Black 2015

Knight Black Horse 2015 (Lychee Sweet)

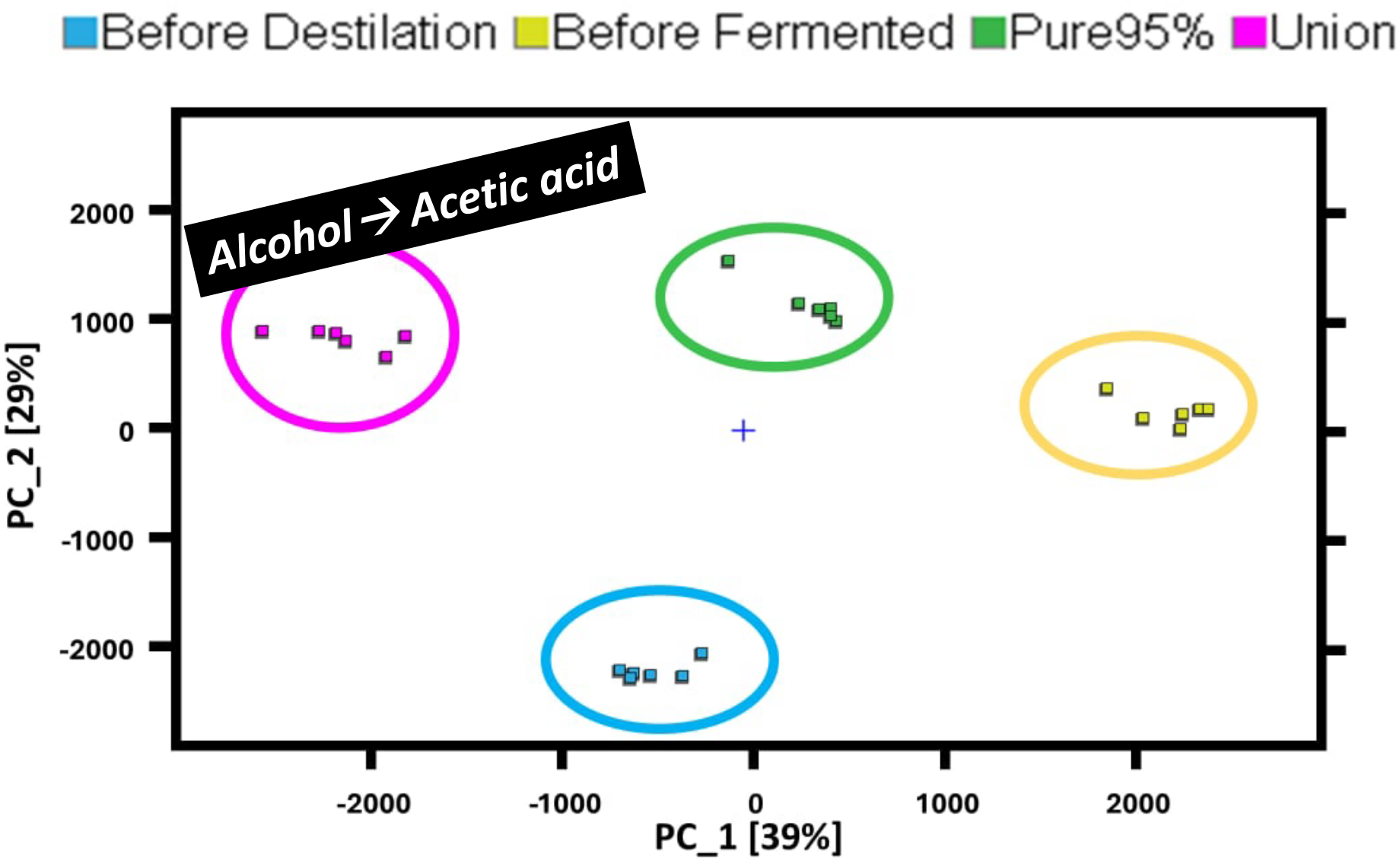
Knight Black Horse 2014 (Mangosteen)





GC-IMS for analysis of volatile organic compounds in alcohol samples

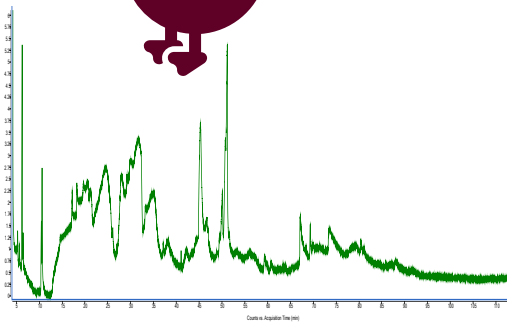
PCA


Before Destilation
Before Fermented
Pure95%
Union
Alcohol → Acetic acid
2000
1000
0
-1000
-2000
PC_2 [29%]
-2000
-1000
0
1000
2000
PC_1 [39%]

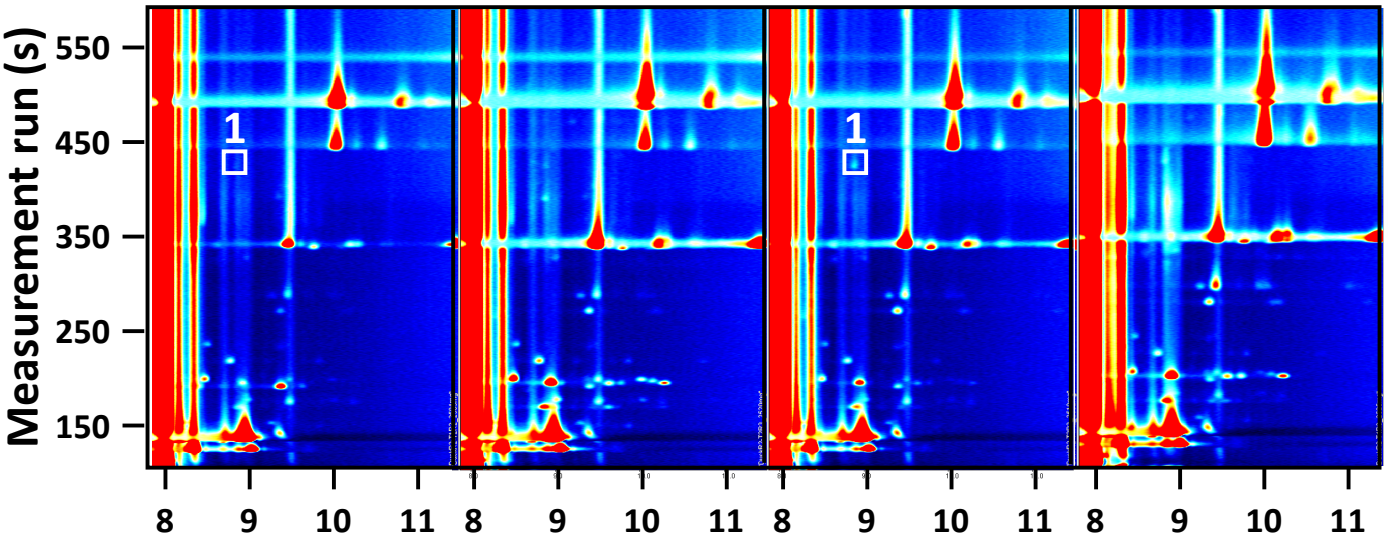
GC-IMS analysis of volatile organic compounds in DUCK samples

GC-IMS application

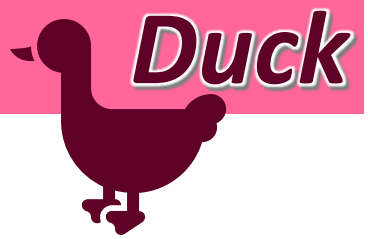
Duck

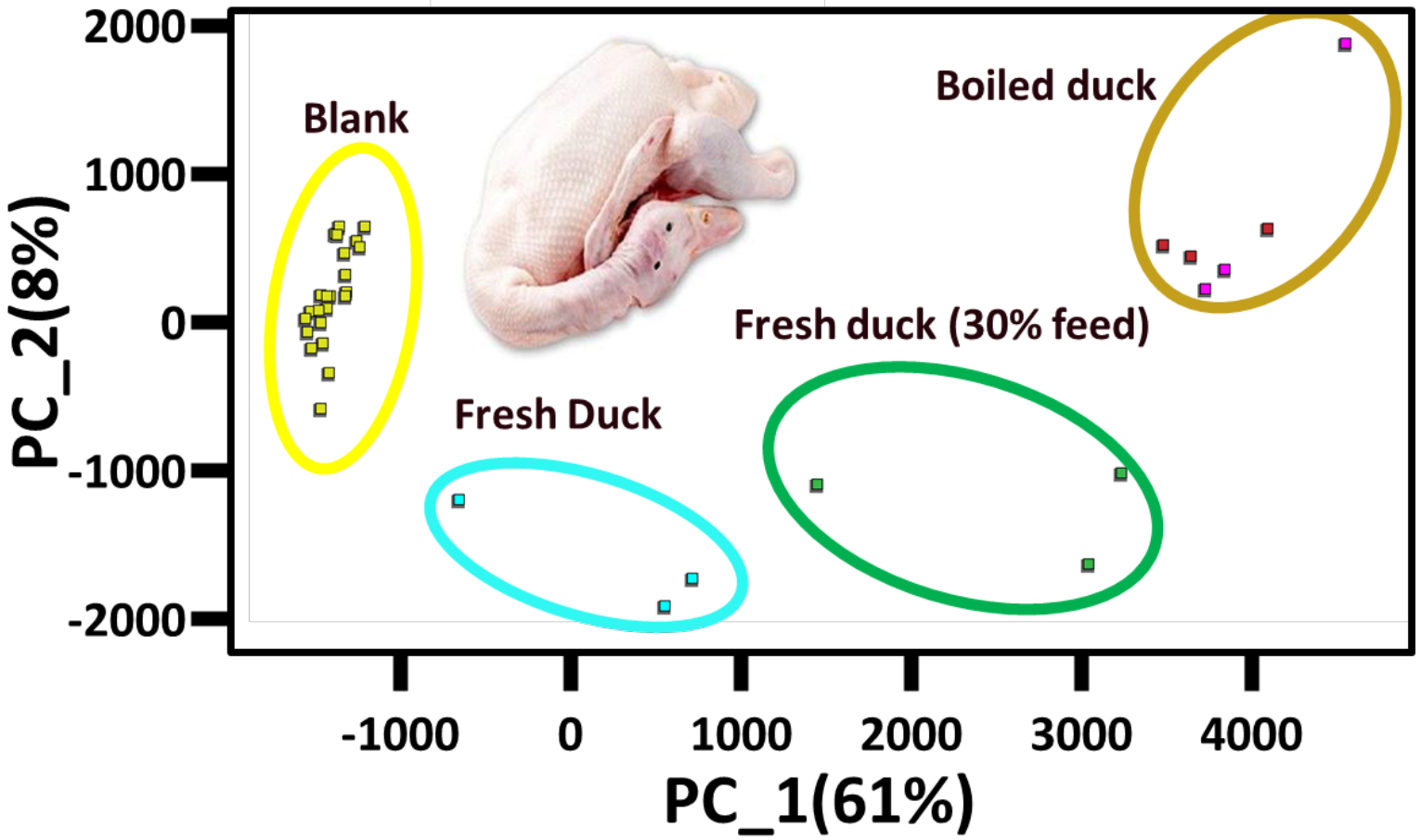


Duck | Boiled Duck | Duck 30% | Boiled Duck 30%



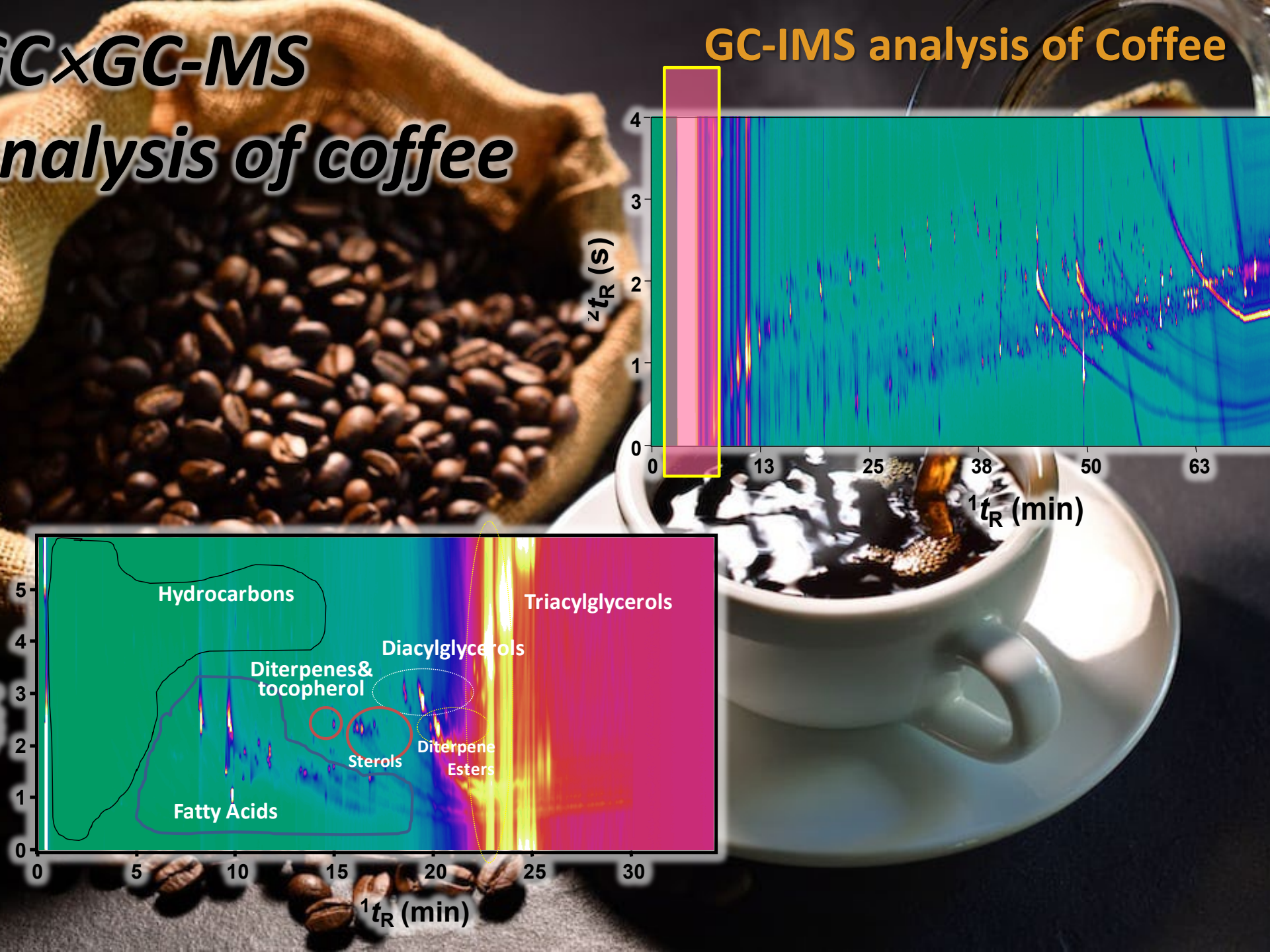
GC-IMS application





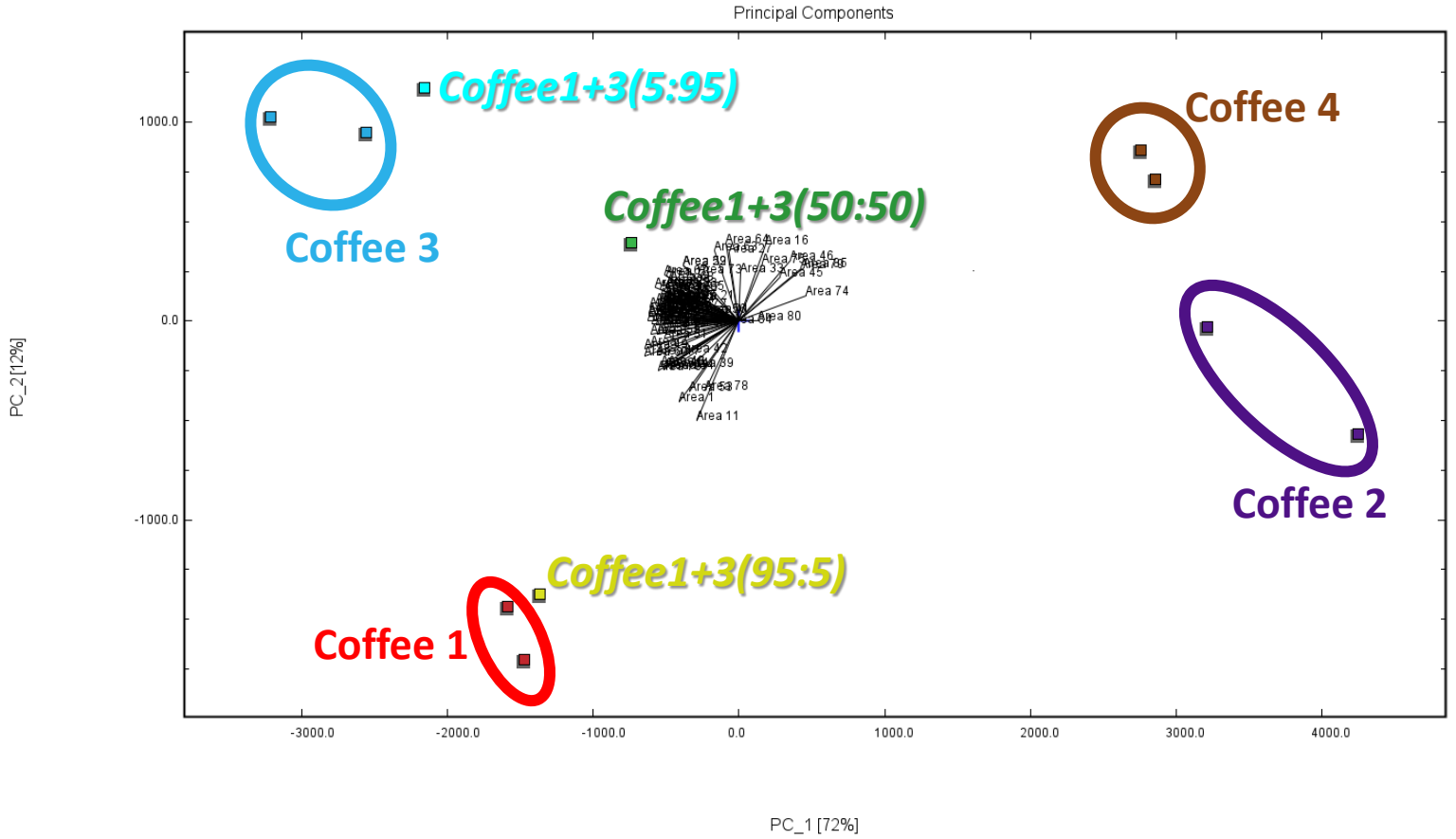
GC×GC-MS analysis of coffee

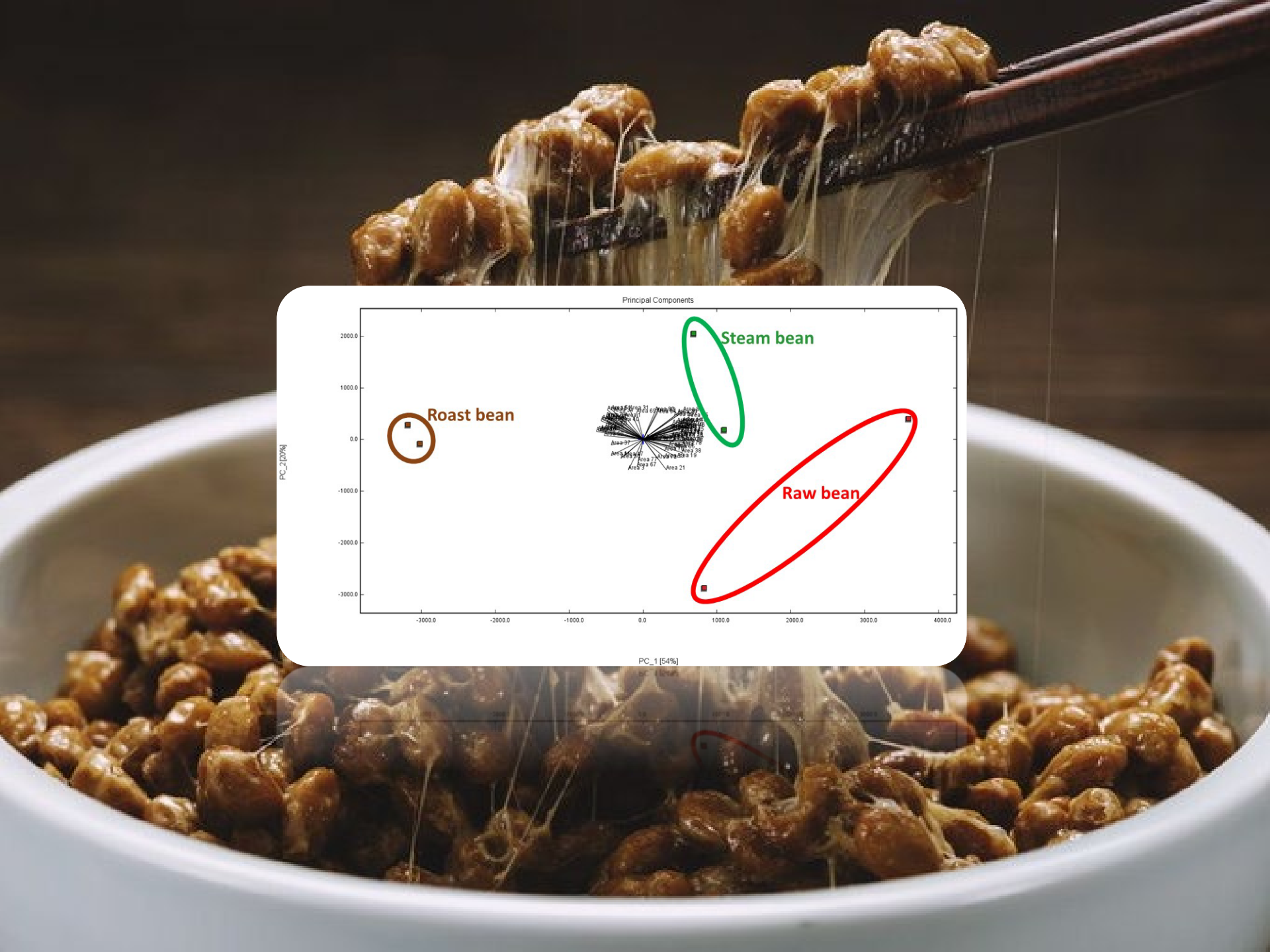
GC-IMS analysis of Coffee



GC-IMS analysis of Coffee

PCA




Principal Components
Steam bean
Roast bean
Raw bean
PC_2 [20%]
PC_1 [54%]
2000.0
1000.0
0.0
-1000.0
-2000.0
-3000.0
-3000.0
-2000.0
-1000.0
0.0
1000.0
2000.0
3000.0
4000.0

Acknowledgement

- Dr Nuttanee Tungkijanansin

Thank You