SENSORY QUALITY OF WINE JUDGED BY ANALYTICAL TECHNIQUES

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Wine Analysis - Overview

- Quality of Wine
- Relevance of Aroma Fingerprinting
- Comprehensive GCxGC-MS
- Identifying Specific Aroma Compounds
- Enhancing Selectivity and Sensitivity

Parameters Affecting the Wine Quality

- **Determining factors**

  - Grape variety
  - Grape ripeness
  - Soil-composition and water supply
  - Climate
  - Yield
  - Fermentation

  (single yeast strain vs spontaneous)

  - Technology

  (reductive, oxidative, stainless steel, barrels)

  - Ageing

Aroma Compounds

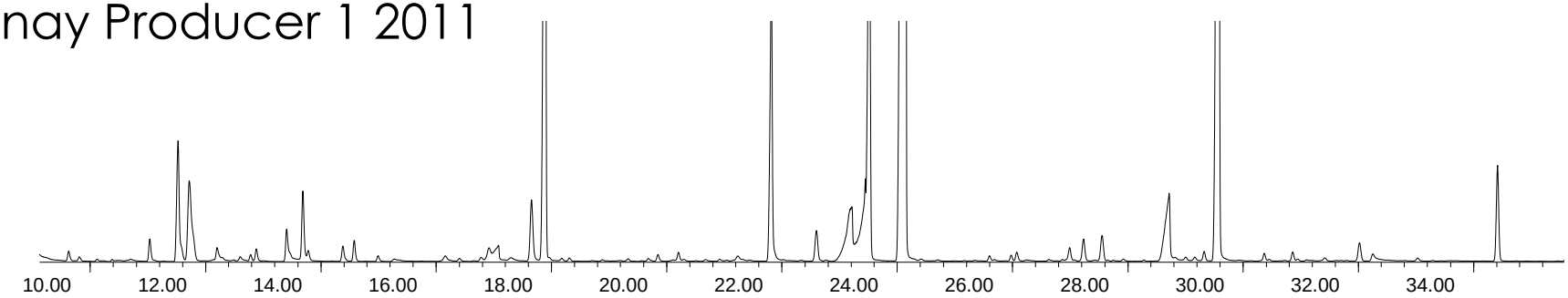
– varietal compounds, either free forms or those obtained from precursors present in grapes
Rotundone, Isobutylmethoxypyrazine, Monoterpenes e.g. Linalool, sulfur compounds

– compounds formed during winemaking that are essentially fermentative compounds

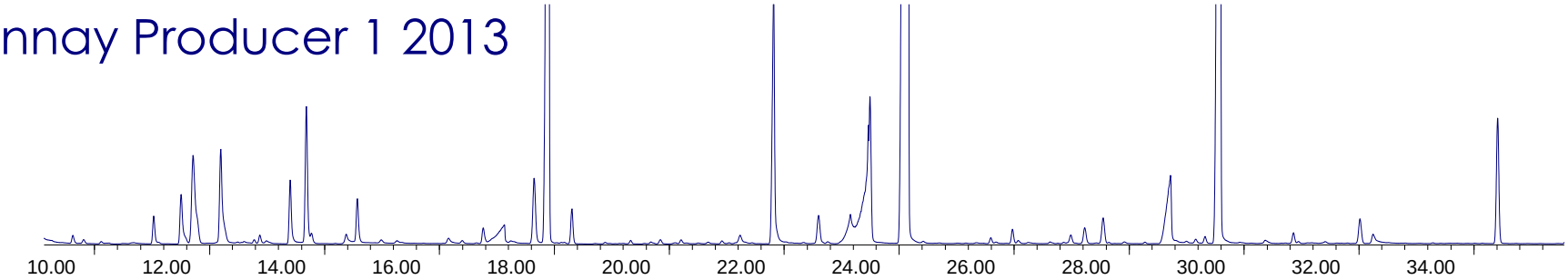
– compounds formed during the maturation of wines

Aromaprofile

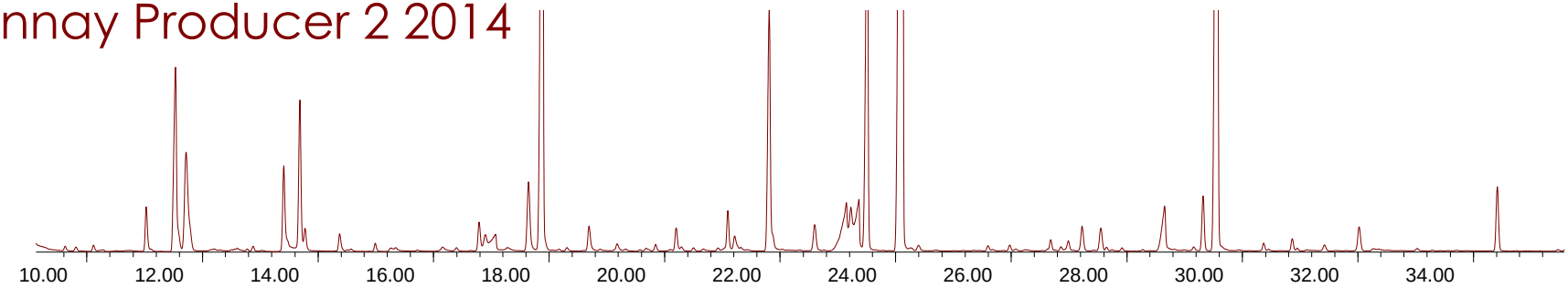
Chardonnay Producer 1 2011



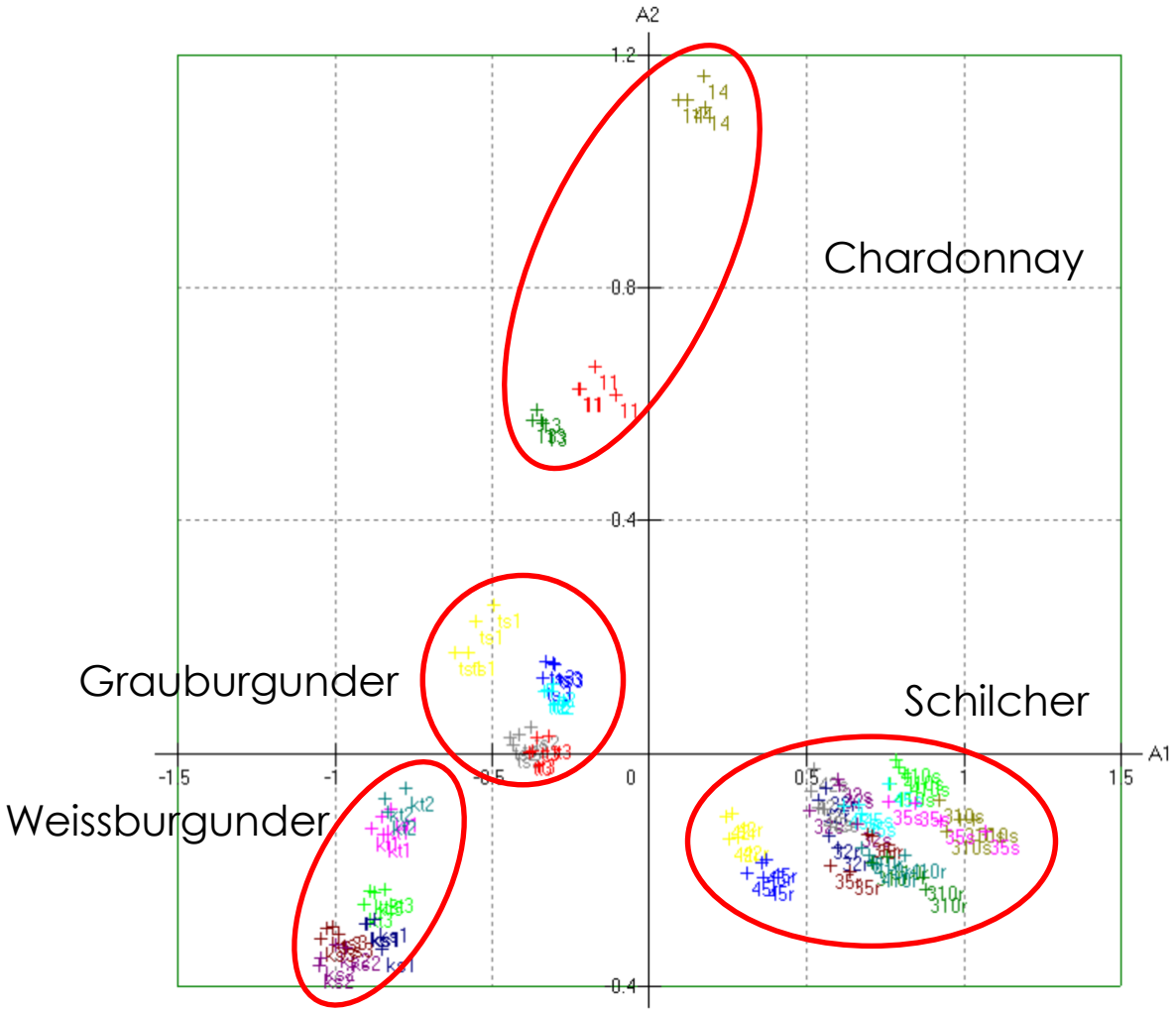
Chardonnay Producer 1 2013



Chardonnay Producer 2 2014

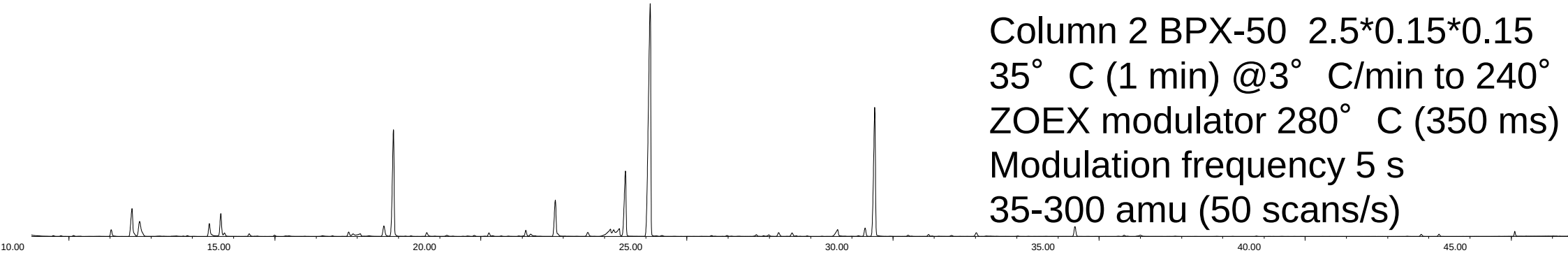


Statistical Analysis

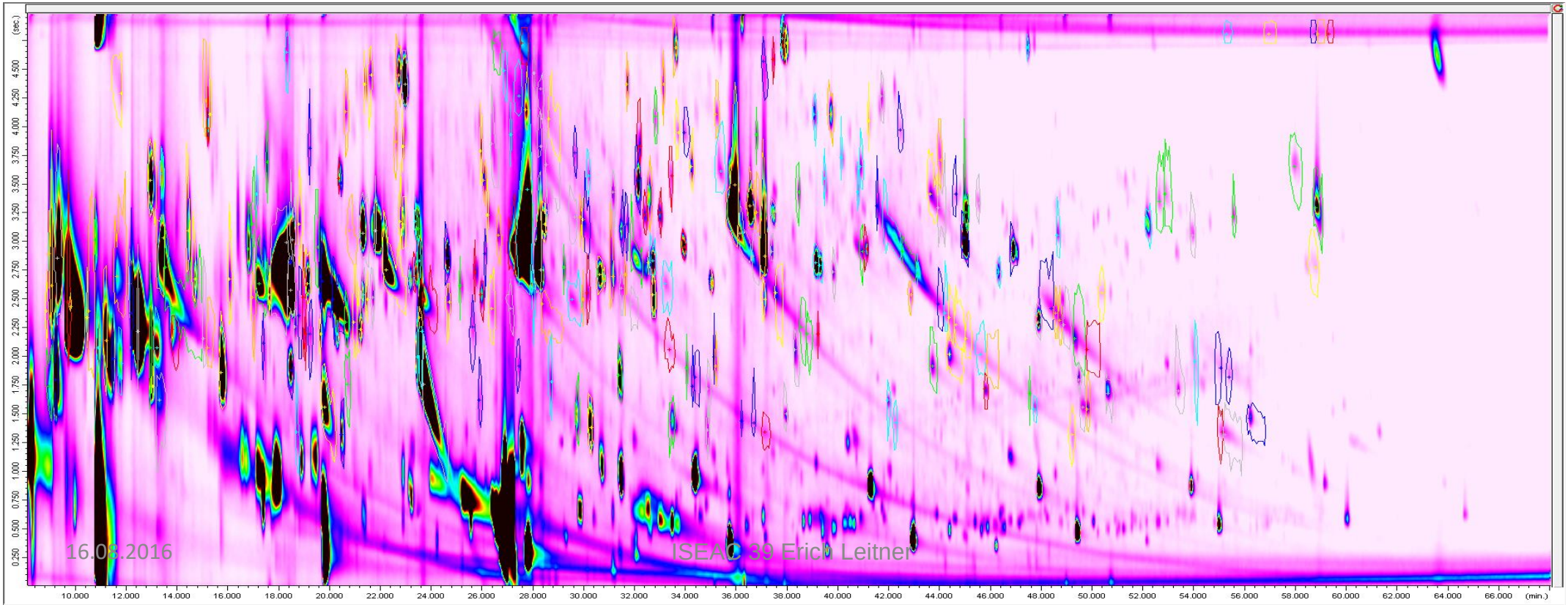


Statistical Analysis can be helpful in the differentiation of different grape varieties and/or vinification processes

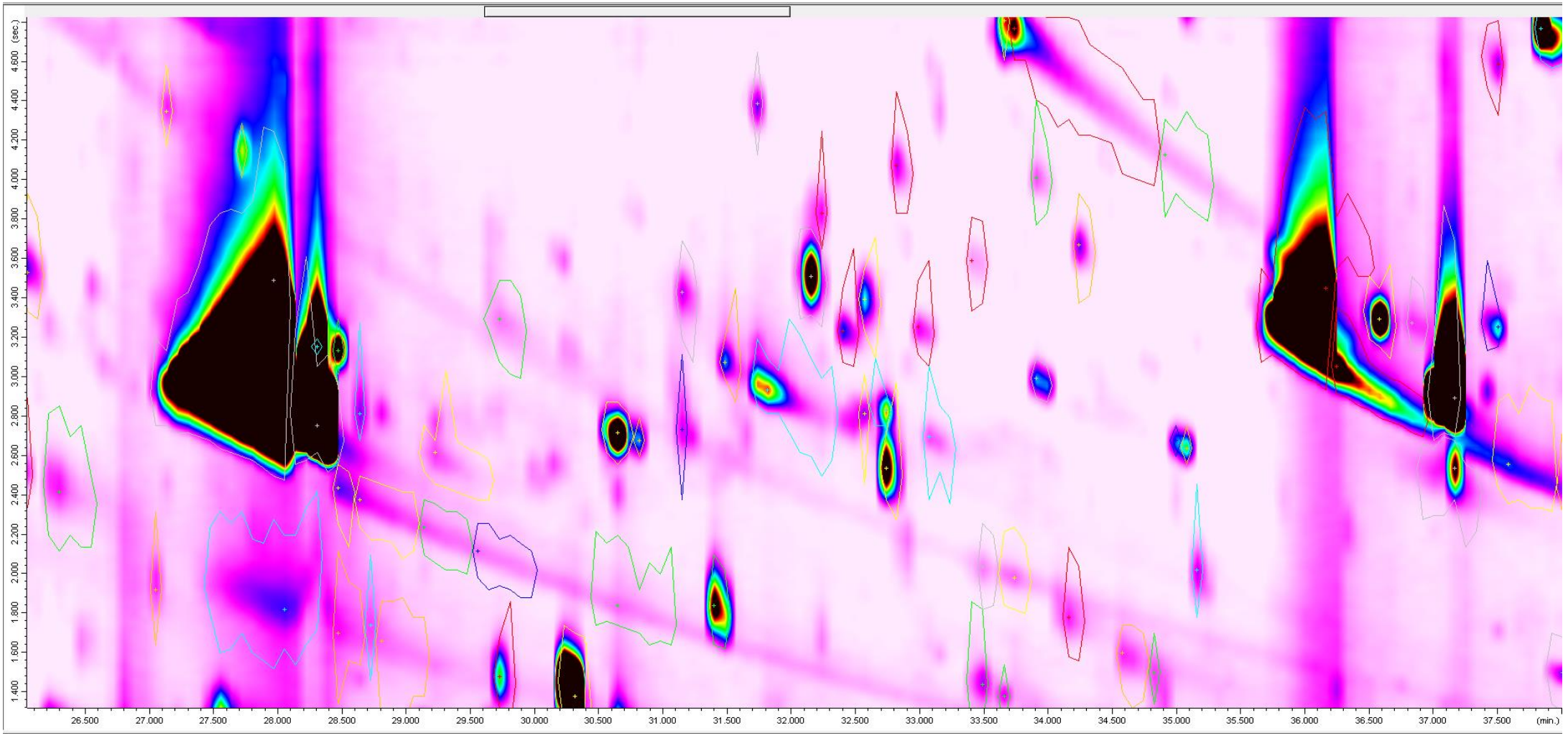
Comprehensive GCxGC-MS



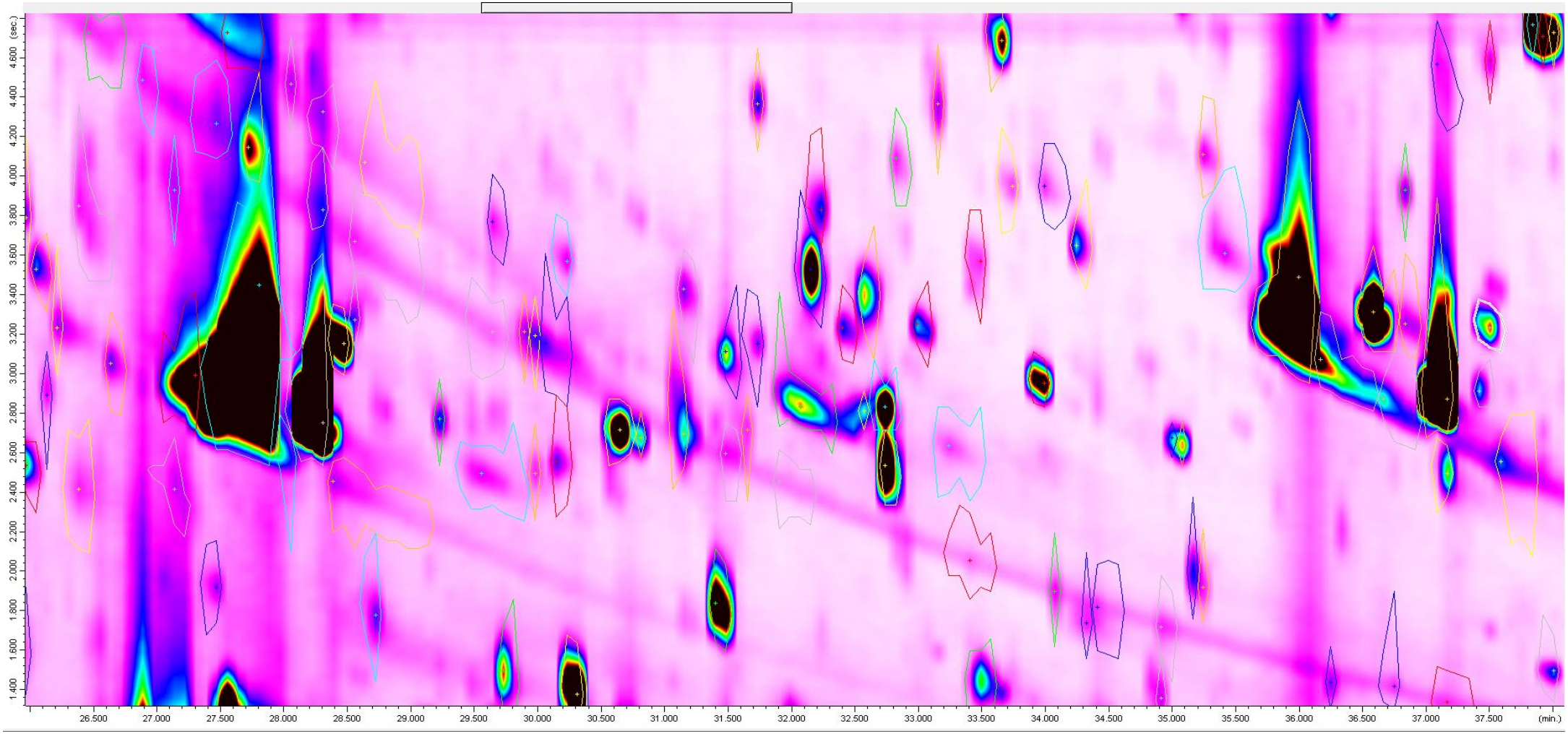
Shimadzu QP2010 plus
Column 1 ZB-1 HT 30*0.25*0.25
Column 2 BPX-50 2.5*0.15*0.15
35°C (1 min) @3°C/min to 240°
ZOEX modulator 280°C (350 ms)
Modulation frequency 5 s
35-300 amu (50 scans/s)



Chardonnay Producer 1 2011



Chardonnay Producer 2 2014



The Molecular Signature of Smell

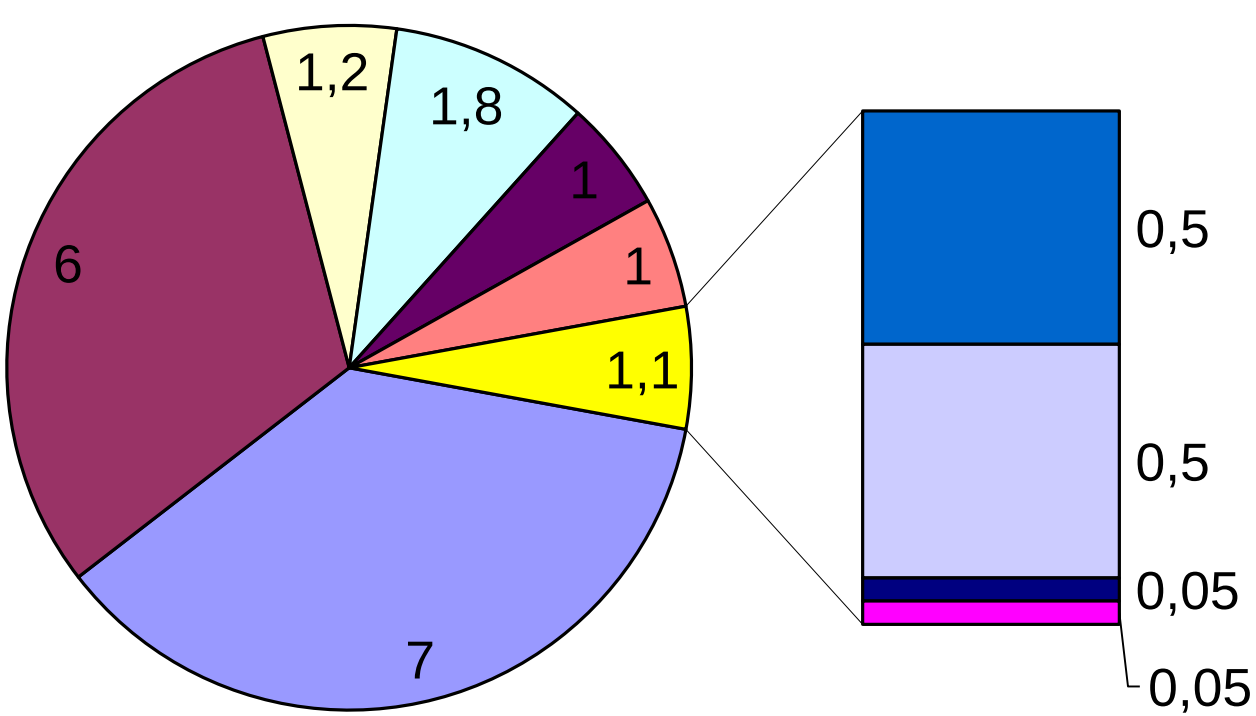
- ***„For mixtures containing more than four components, the odorants were found to lose their individuality and produce a new odor percept conveying a unique odor quality not elicited by the single components.“***

3-40 individual odorants determine the typical smell of a product

Less than 3% of the volatile fraction show odour activity

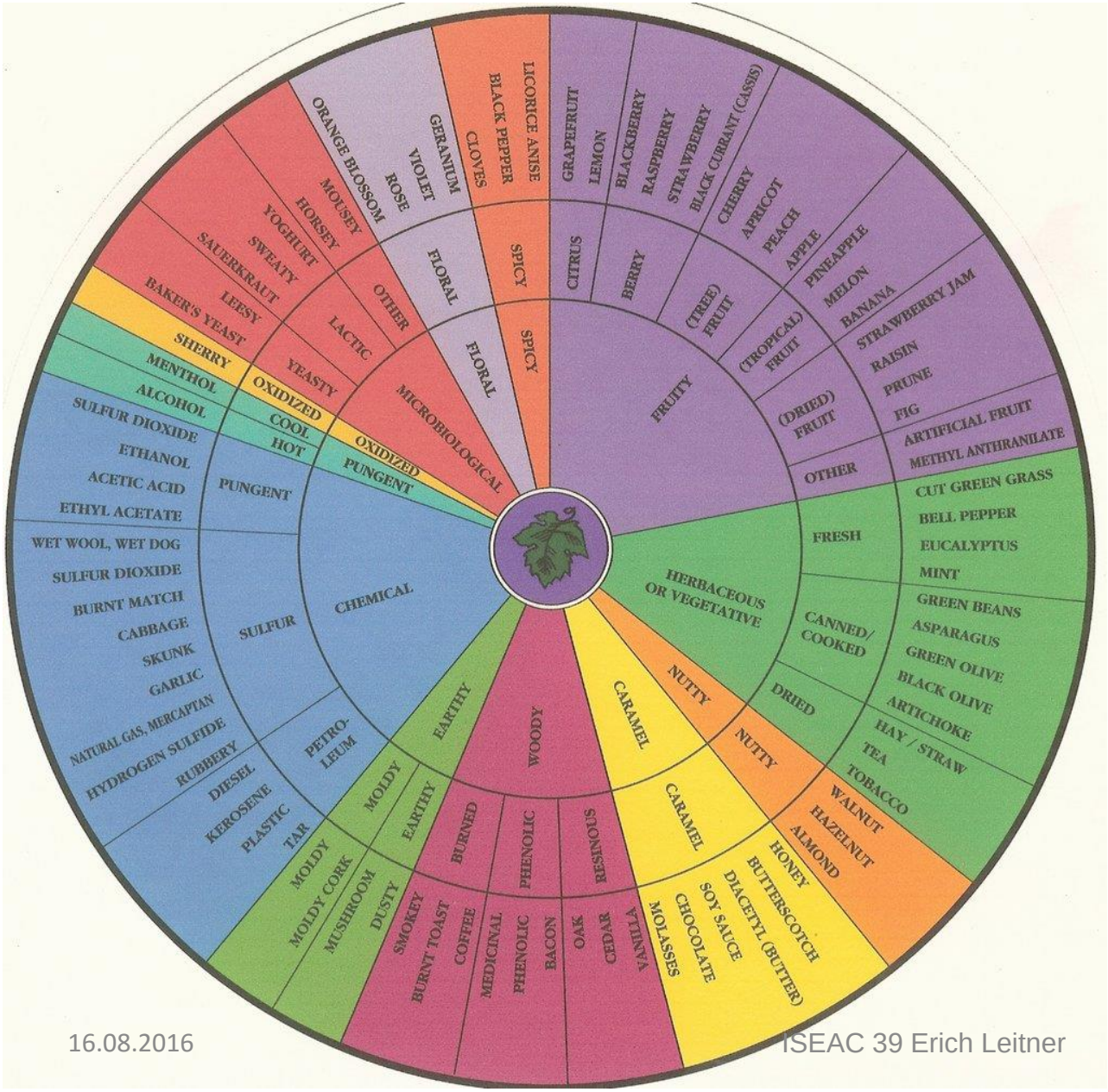
Th. Hoffmann et al,
Natures Chemical Signatures in Human Olfaction: A Foodborne Perspective for Future Biotechnology, Angew. Chem. Int. Ed. 2014, 53, 7124 – 7143

Minor Constituents [g/L]



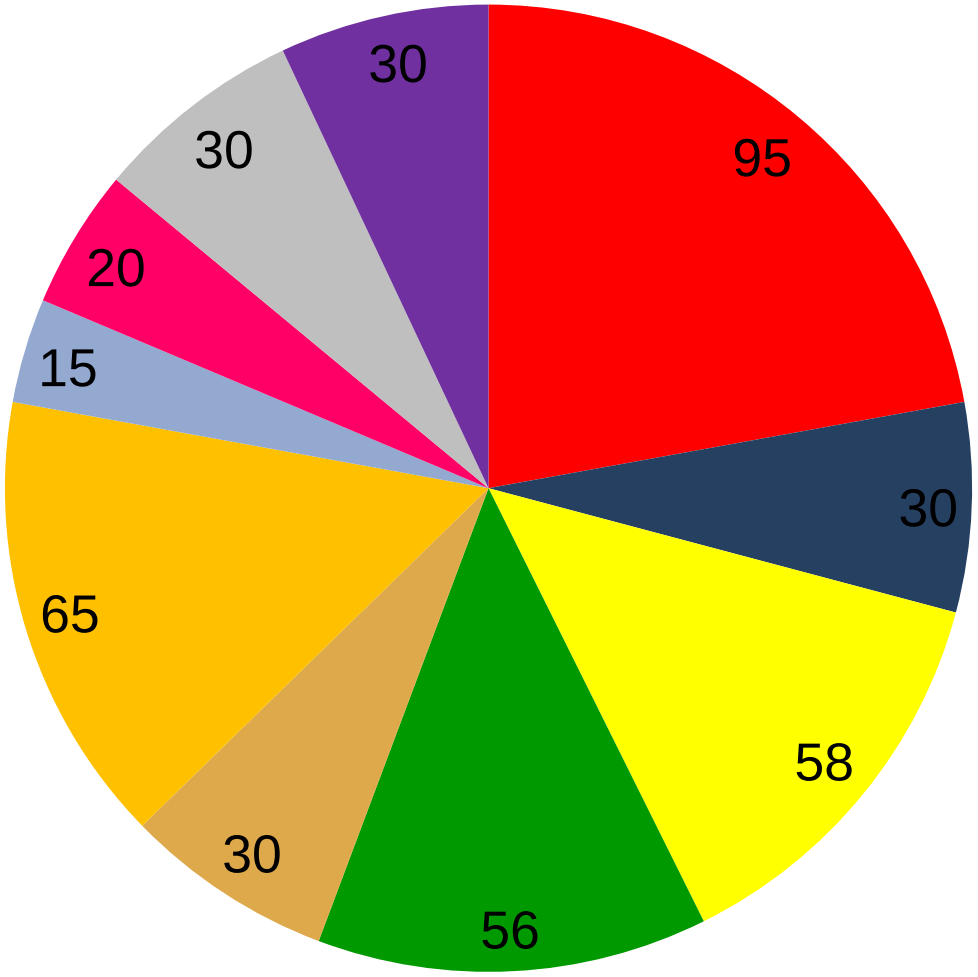
- Glycerol
- Acids
- Minerals
- Non volatile phenols
- Sugar
- Acetic acid
- Higher Alcohols
- Amino acids
- SO2
- Aroma

The Aroma Wheel



Ann Noble UC Davis

The Aroma Compound Wheel



- Ester
- Acids
- Alcohol
- Terpenes
- Carbonyls
- Sulfur Compounds
- Lactones
- Furanes
- Volatile Phenols
- Other

The Concentration Ranges

Compounds	Concentrations [µg/L]
Esters	10-5000
Acids	20-4000
Alcohols	20-1000
Terpenes	0.01-800
Carbonyls	0.1-3000
Sulfur Compounds	0.01-300
Lactones	10-1500
Furanes	20-700
Volatile Phenols	30-3500
Other	0.0008-80

Analytical methods covering the whole concentration range are required!!!

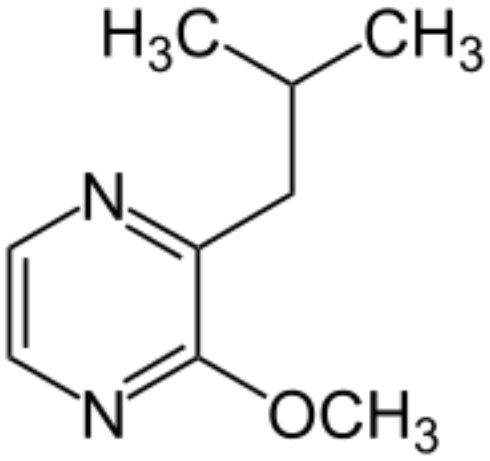
Aroma Compounds in Wine and Threshold

Compound	Aroma descriptor	Concentration in wine [µg/L]	Sensory threshold [µg/L]
Diethyl sulfide	Cooked vegetable	4-32	0.93
Z Oak lactone	Coconut, flowery	n.d.-589	67
4-Ethylphenol	Medicinal, horse sweat	n.d.-6500	140
Ethyl butanoate	Floral, fruity	10-180	20
Ethyl hexanoate	Green apple	30-3400	50
Acetic acid [mg/L]	Vinegar	110-1150	280
Ethyl acetate [mg/L]	Nail polish, fruity	22.5-400	7.5

Bartkowsky E.J., Pretorius I.S., in Biology of Microorganisms on Grapes, in Must and in Wine, Springer Verlag 2009, ISBN 978-3-540-85462-3

The Odour Activity Value (OAV) and NOT the concentration is relevant!!!!!!!!!

Varietal Aroma
2-Isobutyl-3-methoxypyrazine



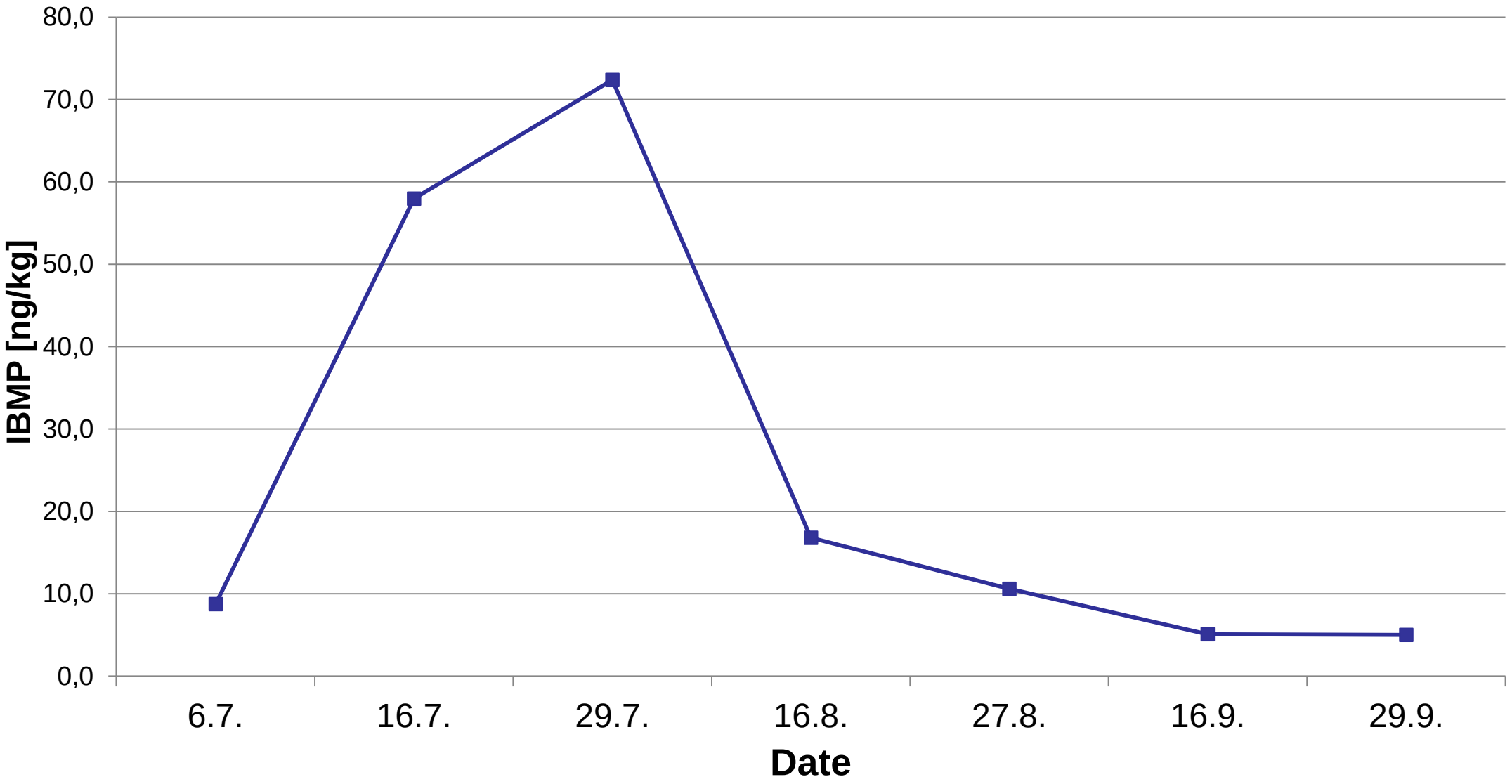
Initially identified in Cabernet Sauvignon grapes, also found in Cabernet Franc, Merlot and Sauvignon Blanc

Sensory threshold: 2ng/L

Odour descriptors: green bell pepper, green gooseberry, aparagus, vegetal

Survives the fermentation and is stable in the wine

Changes of IBMP during *Sauvignon Blanc* Grape Ripening



Quantification using MS/MS with Stable Isotope Dilution Analysis

IS IBMP (d3) 10 ng/L

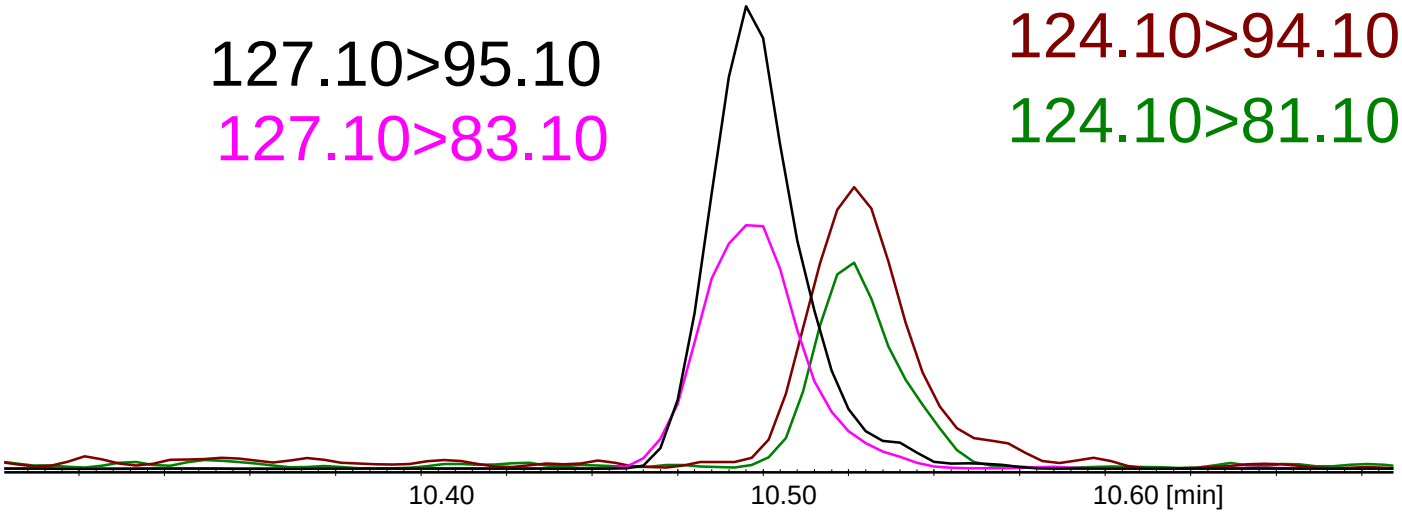
127.10>95.10

127.10>83.10

IBMP 6.1 ng/L

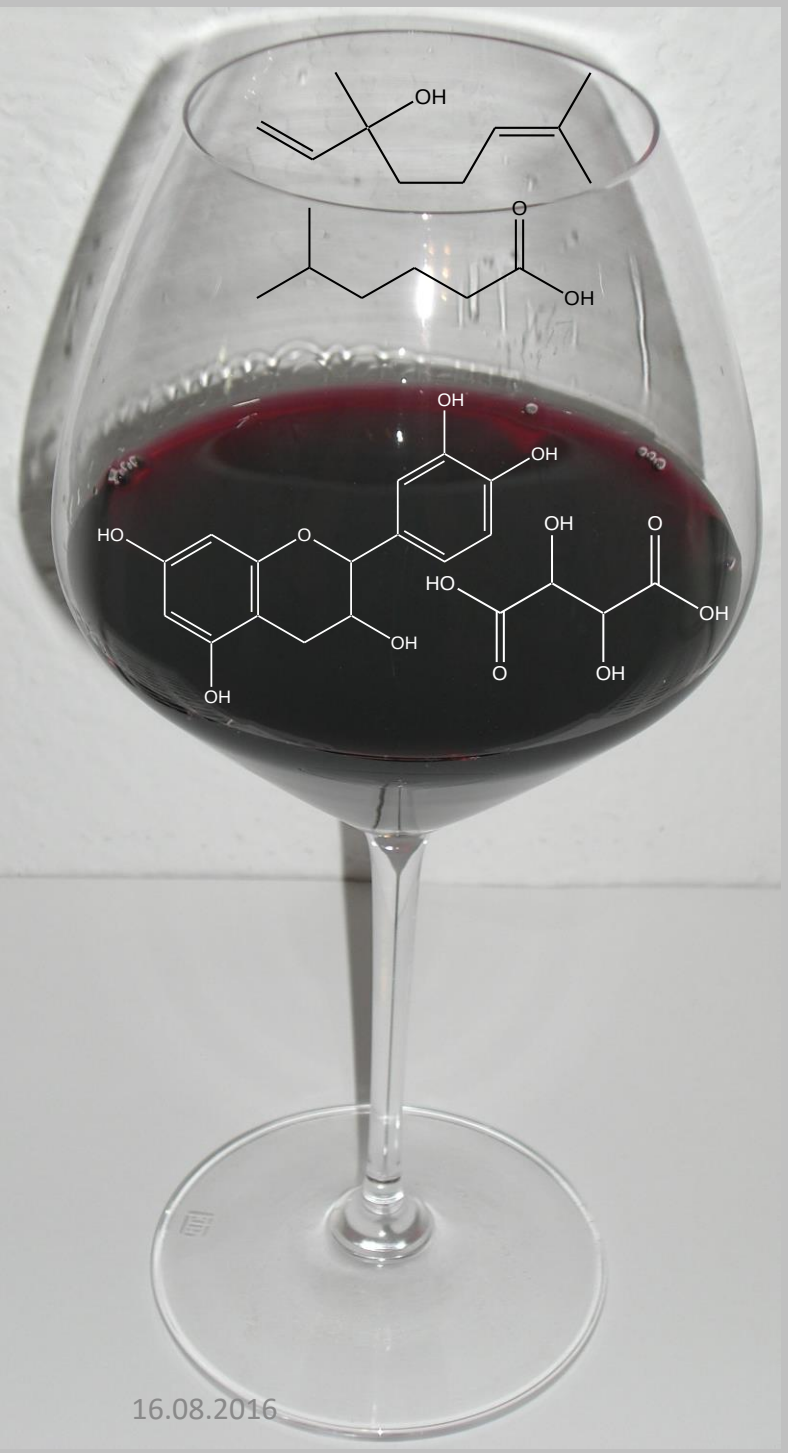
124.10>94.10

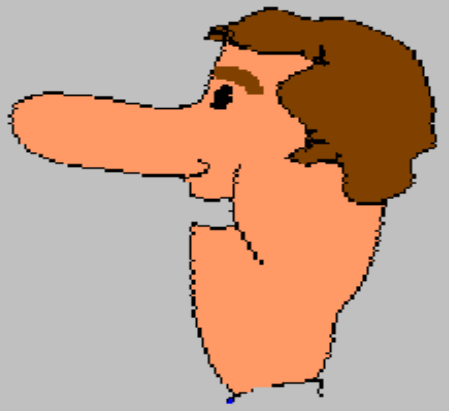
124.10>81.10



Sample preparation: HS-SPME 1 mL, 50/30 µm DVB/Carboxen/PDMS 50° C, 30 min
Shimadzu TQ8040
Column: ZB-5 MS 30*0.25*0.25
Temperature programme: 40° C (1 min) @10° C to 290° C

Substance	Loop Time	Transition	CE	Transition	CE	Transition	CE	Q1 Res	Q2 Res
IBMP-d3	0.1	127.10>95.10	13	127.10>83.10	7	127.10>97.10	11	High	High
IBMP	0.1	124.10>94.10	11	124.10>81.10	7	124.10>79.10	23	High	High





…..thank you for your attention