Modelling of flavour quality in red raspberry

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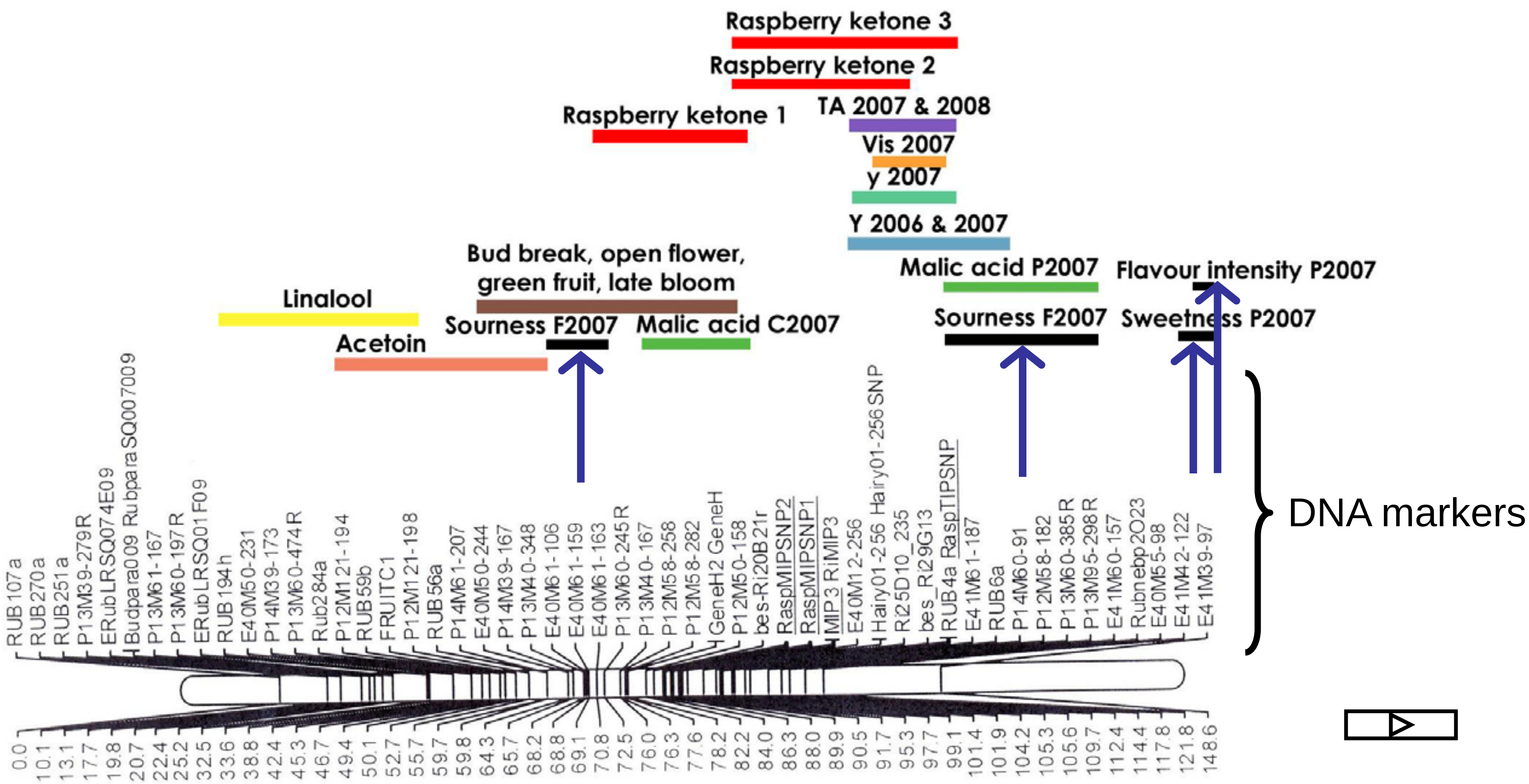
Introduction: Marker assisted breeding

- Flavours in fruit are continuous genetic traits.
- Trait intensity can be linked to DNA polymorphisms (markers)- **quantitative trait loci (QTL)**.

- Polymorphic DNA markers that can be linked to sensory and metabolite content variance.
- Breeding for premium flavour can be accelerated by QTL screening of seedlings before fruiting.

- Relationships of metabolite content to key flavour characters?

Red raspberry QTLs for flavour sensory quality



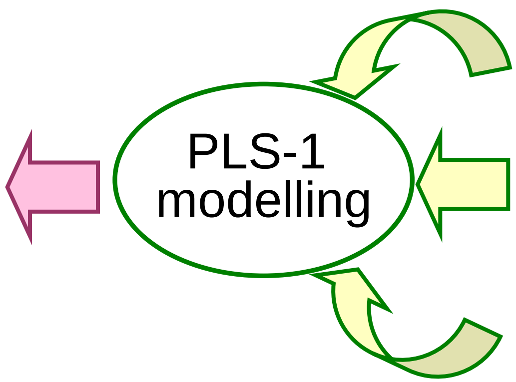
Red raspberry

- Key Scottish fruit crop with nutraceutical benefits.
- Repeat purchase by consumers require consistent flavour quality.
- An improvement strategy is Marker Assisted Breeding for flavour.

Fruit flavour quality

1. Transport / accumulation of **metabolites.**
2. Determined by environment (e.g. season, open vs. covered cultivation) and genotype

Key **metabolites**

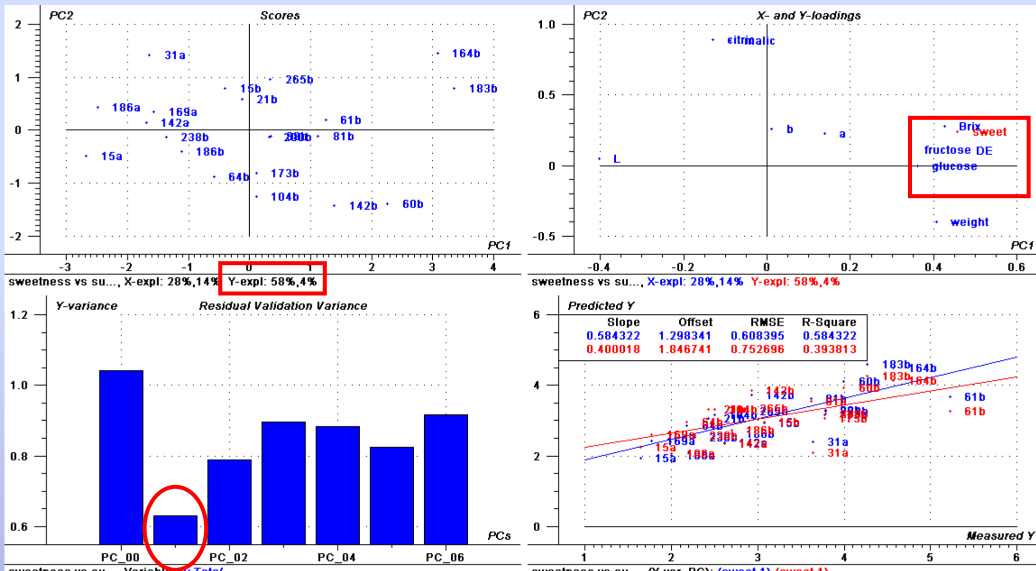


- *Independent variables*- Metabolites content & physical traits (berry size and ^{o}Brix)
- *Dependent variables*- Sensory scores**: sweetness, sourness, flavour intensity**
- *Independent variables*- Impact compound- raspberry ketone

Hypotheses:

- Sweetness, sourness and flavour intensity have complex relationships with fruit metabolites.
- Sweetness does not directly correlate to sugars content.
- Sourness does not directly correlate to acids content.
- Flavour intensity has contributions from volatile metabolites.
- Covered cultivation influences flavour characters in fruit.

PLS-1 model: Physical traits, non-volatile metabolites contents and sweetness sensory scoring



- 62% variation in sweetness accounted for by PC1
- Sweetness driven by:
  hexoses
  ºBrix total solubles (TSS)
  Colour difference, esp. **ΔE**

Figure 1(a): PLS1 model:

Independent variable- Sugars/ acids content, colour meter values and ºBrix total soluble solids

Dependent variable- **Sweetness**

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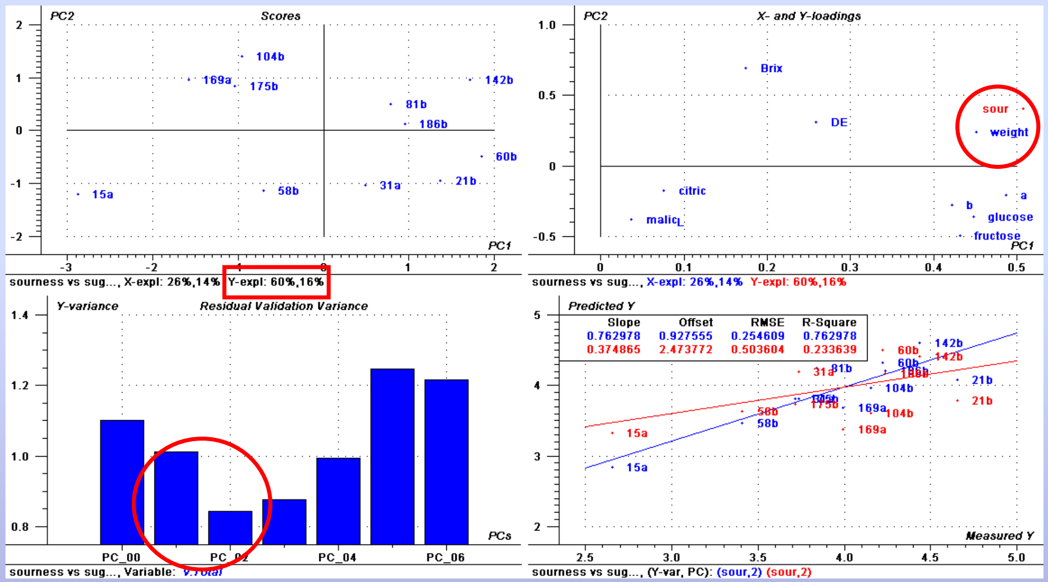
PLS-1 model: Physical traits, non-volatile metabolites content and sourness sensory scoring



- 76% variance in sourness accounted by PC1 &PC2
- Sourness is driven by: **10-berry weight** (water content)
- **Hexoses** have stronger effects than organic acids content on sourness scoring

Figure 1(b): PLS1 model:

Independent variable- Sugars/ acids content, colour meter values and °Brix total solids

Dependent variable- **Sourness**

PLS-1 model: Physical traits, non-volatile metabolites content and flavour intensity sensory scoring

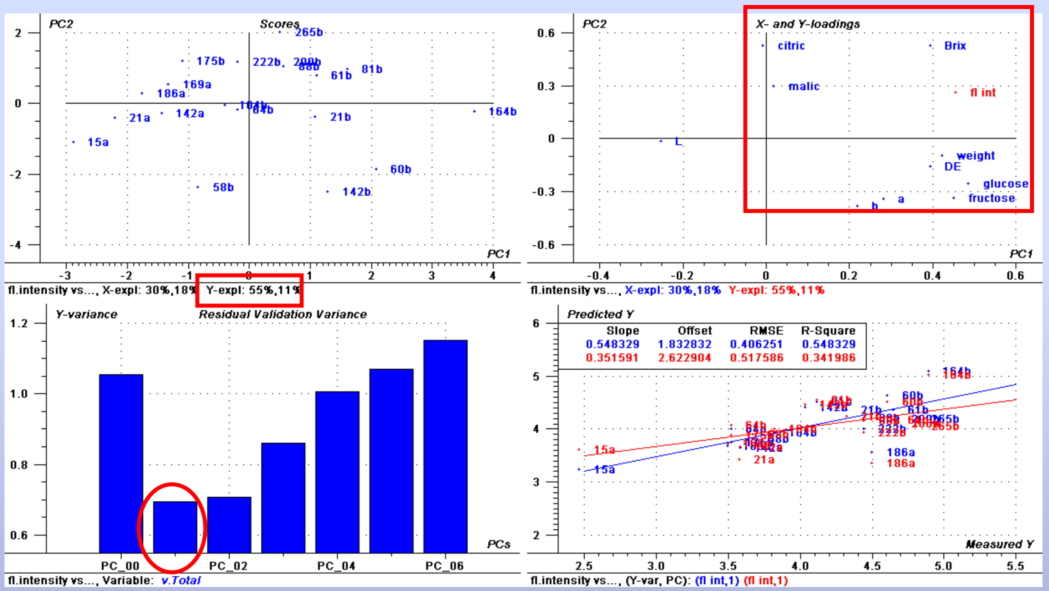


Figure 1(b): PLS1 model:

Independent variable- Sugars/ acids content, colour meter values and ºBrix total solids

Dependent variable- **Flavour intensity**

- 66% variation in flavour intensity accounted by PC1
- Flavour intensity is driven by:
  ºBrix (total solubles)
  hexoses
  organic acids
  10-berry weight (water content)

  Colour difference (ΔE), green-red (a) and blue-yellow (b) spectra are good predictors.

Conclusion

PLS-1 models: Physical traits, non-volatile metabolite contents and sensory scoring

(a) Common drivers for all sensory scoring models:
- **Sugars**
- **Water content** (berry weight)
- **Colour** (pigmentation)

(b) Instrumental correlations with sensory scoring:
- **ºBrix** (TSS content)
- certain **colour meter values**

(c) **Non-linear relationships**
-metabolites enhancing and muting more than a single sensory trait.

(d) Complex relationships between sensory scores, affected by:
- **Quantities** of metabolites in fruit cells
- **Sensory interactions** in assessors in scoring

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PLS-1 model: Volatile and non-volatile metabolites and sweetness sensory scoring

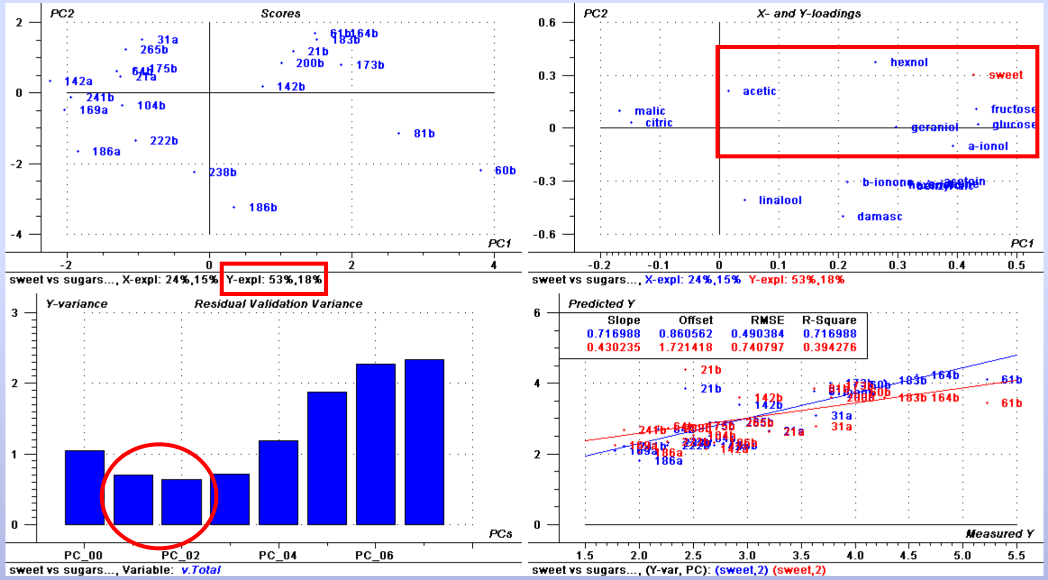


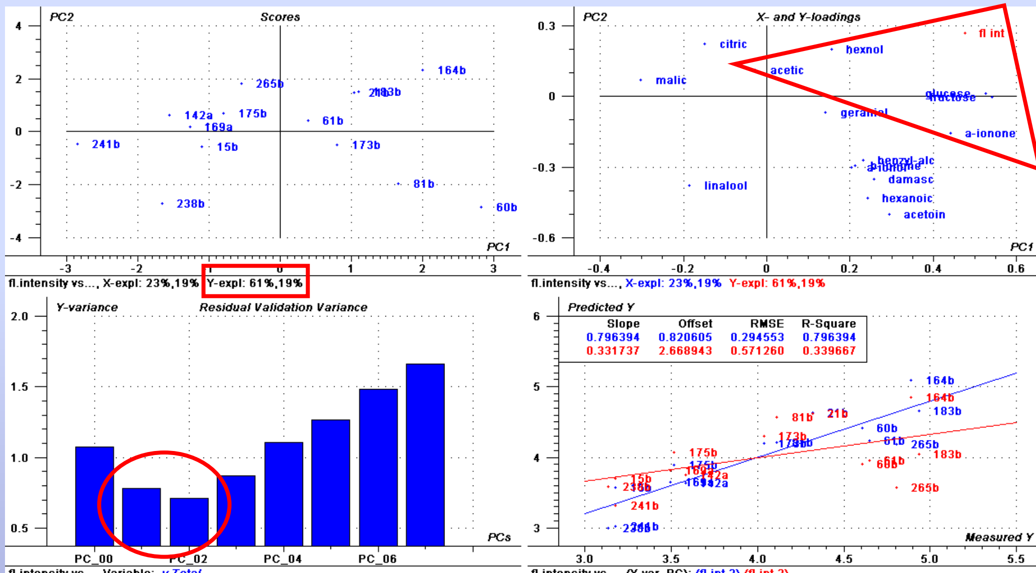
Figure 2(a): PLS1 model:

Independent variable- Sugars/ acids & volatiles content

Dependent variable- **Sweetness**

- 71% variance in sweetness accounted by PC1 and PC2
- Sweetness driven by hexenol, geraniol, α-ionol, acetic acid. These volatiles increase effect of hexoses on sweetness.

PLS-1 model: Volatiles and non-volatiles metabolites and flavour intensity scoring



- 80% variance in flavour intensity scores accounted by PC1 and PC2
- Flavour intensity driven by: hexenol, α-ionone. These volatiles increase effect of hexoses on flavour intensity.

Figure 2(b): PLS1 model:

Independent variable- Sugars/ acids and volatiles content

Dependent variable- **Flavour intensity**

Note: There is no adequate models to describe correlations between volatile contents and sourness

Conclusion

PLS-1 models: Volatile & non-volatile metabolite contents and sensory scoring

- Adding volatiles content improve modelling on sensory scoring.
- Important volatile driver of flavour- **hexenol**,
  Increases effect of **hexoses** on *sweetness* and *flavour intensity*.

- Sensory characters are not only accumulation of non-volatiles,

- There are sensory interactions of volatiles and non-volatiles in human assessors.

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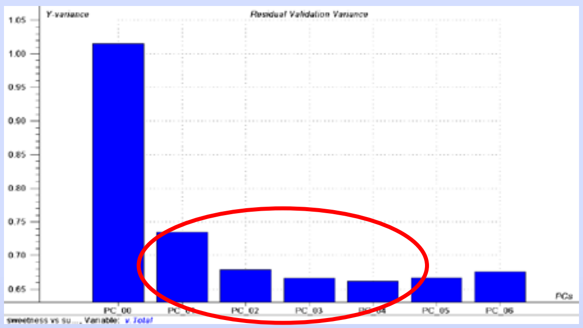
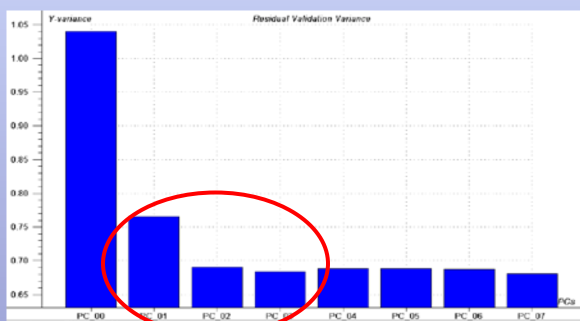
PLS-1 model: Physical traits, non-volatile metabolites, raspberry ketone and sweetness sensory scoring



Without RK,Y-explained, 41%



With RK,Y-explained, 42%

- **1%** increase in sweetness scoring variance

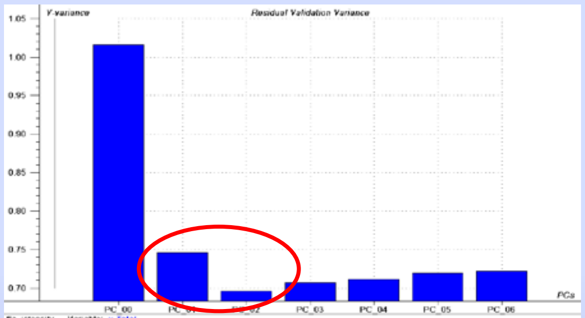
Changes in model contribution: (β-coefficients) for multiple variables

- Increases effects of **hexoses**, **10-berry weight**, **colour difference (ΔE)**

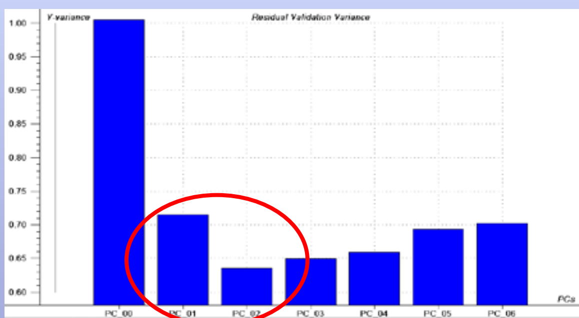
- Decrease effects of: **ºBrix** (TSS content), **malic acid**, **total acids**

Variables	β-coefficients		
	Without RK	With RK	
Fructose	-3.190e-02	4.239e-02	↑
Glucose	0.138	0.152	↑
Total sugars	8.030e-03	7.069e-02	↑
Citric Acid	-3.588e-02	-1.580e-02	↑
Malic Acid	0.101	7.849e-02	↓
Total Acids	1.110e-02	5.839e-03	↓
ºBrix	0.555	0.433	↓
Weight	8.668e-02	0.164	↑
L*	-4.408e-02	-3.904e-02	
a*	3.119e-03	3.417e-02	
b*	-4.653e-03	2.831e-02	
ΔE	5.563e-02	6.496e-02	↑
RK	-n/a-	1.882e-02	

PLS-1 model: Physical traits, non-volatile metabolites, raspberry ketone and flavour intensity sensory scoring



Without RK,Y-explained, 40%



With RK,Y-explained, 45%

Note: There is no adequate model to describe correlation between RK content and sourness

- **5%** increase in flavour intensity scoring variance, same PC #, reduced variance explained by each PC.
- Increases effects of: **hexoses**, **citric acid**, **10-berry weight**, certain **colour meter values**
- Decreases effects of: **malic acid**, **total acids**, **ºBrix** (TSS content)

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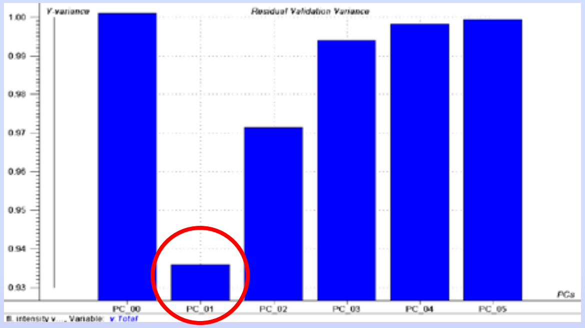
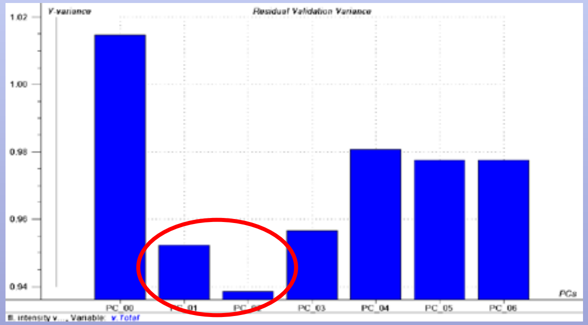
PLS-1 model: Volatile metabolites, raspberry ketone and flavour intensity sensory scoring



Without RK,Y-explained, 21%



With RK,Y-explained, 19%

- Variance in flavour intensity scoring reduced by 2%,
- Increases effects of: **Linalool**, **Benzyl-alcohol**, **Hexenol**, **Hexanoic acid**.
- Decreases effects of: **β-damascenone**, **Geraniol**, **α-** and **β-ionone**, **α-ionol**, **Acetic acid**, **Acetoin**

Variables	β-coefficients		
	Without RK	With RK	
Linalool	-4.802e-02	-2.880e-02	⇧
β-damascenone	3.915e-02	7.267e-03	⇩
Geraniol	9.408e-02	8.402e-02	⇩
α-ionone	0.145	0.132	⇩
β-ionone	0.175	0.132	⇩
Benzyl alcohol	-2.614e-02	-1.392e-02	⇧
α-ionol	-6.542e-04	-4.785e-02	⇩
Acetic acid	-2.238e-02	7.994e-03	⇩
Hexenol	-0.135	-0.149	⇧
Acetoin	6.681e-02	3.575e-02	⇩
Hexanoic acid	4.367e-03	-9.899e-03	⇧
RK	-n/a-	4.483e-02	

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Conclusions

PLS-1 models: Raspberry ketone and sensory scoring

- Addition of RK into models:

  - Important aroma volatile-**1- 5% change** in sensory variance
  - **Increases effects of non-volatiles** on sensory scoring
  - **Enhanced** and **muted effects** of certain other volatiles

PLS-1 models: Metabolites and sensory scoring

Complex fruit flavour effect of non-volatiles content:

- Non linear correlations with volatile metabolites
- Interactions between sensory traits
- Sensory interactions in assessor

Multiple factors contribute to fruit sensory variance:

- Metabolic pathways and transport system
- Sensory stimuli not associated to flavour- e.g. colour

Thank you for your attention

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Dr. Angzzas Kassim
Dr. Susan McCallum
Dr. Alistair Paterson &
Dr. Julie Graham