# Coffee Flavour Modulation – Reinforcing the Formation of Key Odorants while Mitigating Undesirable Compounds


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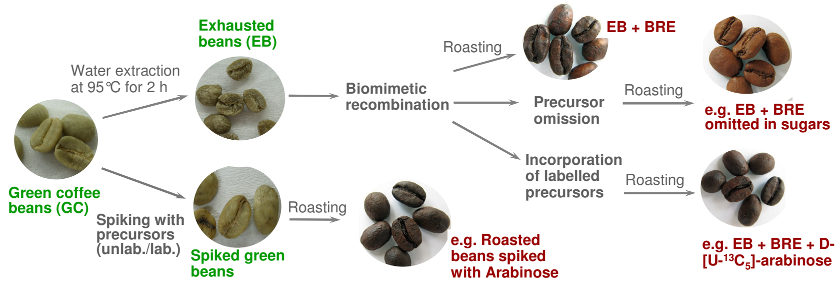
## INTRODUCTION

The formation of important coffee aroma compounds has been extensively studied in model systems under dry heating conditions [1-3]. This has recently been extended to undesirable compounds such as furan [4]. However, the conclusions from results of model systems have to be taken with care and cannot simply be extrapolated to complex food products. Milo et al. [5] developed the so-called biomimetic in-bean experiment in order to study the importance of precursors for the formation of key aroma compounds during coffee roasting under real conditions. Said methodology is a potential tool when it comes to studying the modulation of coffee flavour.

### Objective and Approach

Our study aimed at modulating coffee flavour based on the chemical understanding of formation pathways of character impact aroma compounds such as 2-furfurylthiol (FFT) and pyrazines. In parallel, furan was monitored in order to identify strategies for its mitigation.

A combination of biomimetic in-bean experiments and spiking of green coffee with precursors was implemented. Biomimetic recombination of exhausted beans was based on analytical evaluation of the water extractable composition (Biomimetic recombined extract, BRE).




## RESULTS & CONCLUSIONS

### Model System

#### 2-Furfurylthiol (FFT)

- FFT has been shown to be formed in arabinose/cysteine model systems *via* 3-deoxypentosone and furfural while maintaining the intact carbon chain [1].
- Grosch [2] provided evidence for arabinogalactanes being the precursor of FFT by isolating the polysaccharide from green coffee and roasting it in the presence of cysteine.
- Milo et al. [5] stated that FFT derives from water non-extractable precursors as increased FFT amounts were found in water-extracted exhausted beans.

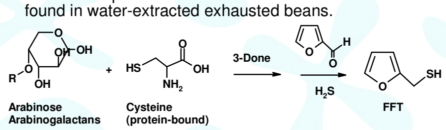



**Figure 1**: Hypothetical formation of FFT in coffee from arabinogalactans or arabinose (R=H) and cysteine (protein-bound).

### In-Bean Experiment

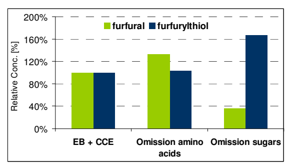



**Figure 2**: Omission experiments (left).

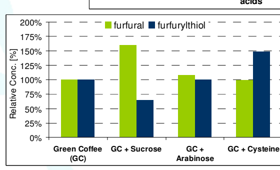



**Figure 3**: Spiking of green coffee with sugars (equimolar amounts) and cysteine.

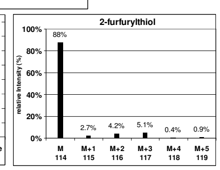



**Figure 4**: Incorporation of D-[U-$^{13}C_5$]-arabinose (16% of natural content).

### Findings

- Formation of FFT in coffee seems not to occur *via* furfural as intermediate compound and involves smaller sugar fractions:
  - Omission of sugars favored the generation of FFT, whereas furfural content was highly suppressed (Fig. 2);
  - Spiking with sucrose (Fig. 3) increased furfural amounts but considerably decreased concentrations of FFT;
  - Incorporation of D-[U-$^{13}C_5$]-arabinose did not yield fully labelled FFT, but partially labelled FFT with $^{13}C_1$, $^{13}C_2$ and $^{13}C_3$-moieties (Fig. 4).
- Spiking experiment (Fig. 3) with cysteine resulting in enhanced FFT amounts show an avenue for coffee aroma modulation.

#### Pyrazines

- Potential precursors are $C_6$ and $C_5$ sugars (e.g. fructose, glucose or arabinose) whose degradation compounds form key intermediates (e.g. α-amino-oxo compounds) through the Strecker reaction [3].
- In addition, alanine and glycine plays a key role as they are integrated into the side chain of the alkyl pyrazine molecule [3].

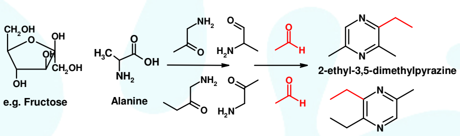



**Figure 5**: Precursors and key intermediates of pyrazines [3].

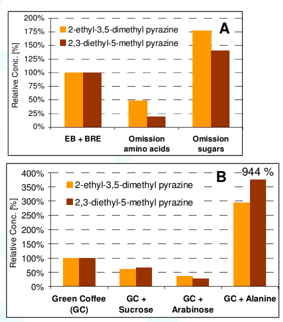



**Figure 6**: Omission experiments (A) and spiking of green coffee with sugars (equimolar amounts) and alanine (B).

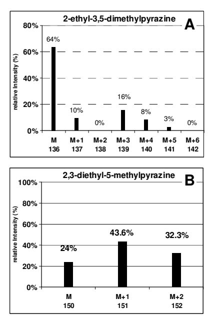



**Figure 7**: Incorporation of [U-$^{13}C_6$fructose]-sucrose (16% of natural content) (A) and spiking with L-[3-$^{13}$C]-alanine (B).

- Amino acids, in particular alanine, are key precursors in the formation of ethyl pyrazines:
  - Omission of free amino acids and spiking with alanine confirmed their importance (Fig. 6);
  - Labelled alanine is efficiently incorporated into the molecule (Fig. 7B).
- Formation of $C_3$-fragments occurs from free sugars as well as from non-water extractable polysaccharides:
  - Sugars omission (Fig. 6A) resulted in highly increased pyrazine concentrations, whereas spiking of green beans with sugars (Fig. 6B) had a suppressing effect;
  - Pyrazine formation implies competition between bound and free sugars for the water extractable N-source.

#### Furan

- Major pathway of furan from arabinose proceeds *via* 3-deoxyosone and furfural as key intermediates [4].
- CAMOLA experiments revealed that furan from hexoses is mainly derived from the intact C3-C4-C5-C6 moiety of the sugar (i.e. glucose) [4].

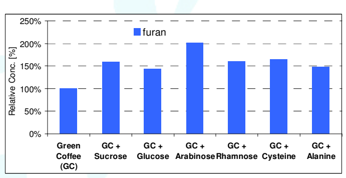



**Figure 8**: Spiking of green coffee with sugars (equimolar amounts) and/or amino acids.

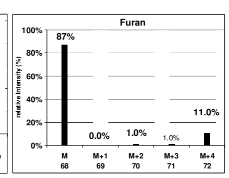



**Figure 9**: Incorporation of D-[U-$^{13}C_5$]-arabinose (16% of natural content).

- Arabinose showed highest potential in generating furan, followed by rhamnose and sucrose (Fig. 8).
- Spiking with labelled arabinose (Fig. 9) verified the direct conversion of the carbon skeleton of arabinose into furan.
- Incorporation of single-labelled alanine into furan was evidenced (results not shown).

### Conclusions

- ✓ The results of the biomimetic in-bean experiments emphasize the potential of this methodology for the verification of proposed formation pathways in complex food systems like coffee and the evaluation of opportunities for aroma modulation.
- ✓ A potential avenue for aroma modulation could be to increase both cysteine and alanine as well as decrease sucrose while mitigating the amount of furan.
- ➢ However, mitigation of furan seems to be limited as both key aroma compounds and furan are formed from common precursors.

## REFERENCES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