The molecular basis of food quality
- The role of polyphenols in coffee -

ACS Award Symposium
San Francisco, 12.08.2014
Imre Blank, Nestlé R&D
Challenges to fill the space between premium quality, health, and convenience

Aroma
Taste
Colour
Crema

Premier quality

Convenience

Instant beverage
Ready-to-drink
Shelf-life

Health & wellness

Stimulating effect on CNS
Antioxidative activity
Chemopreventive activity
Decreased risk of type 2 diabetes
Green coffee composition - Specific constituents make the difference

Great diversity

Robusta

Proteins
Caffeine
Chlorogenic acids
Ash

Limited diversity

Arabica

Saccharose
Lipids
Trigonelline
Organic acids

Average composition of green coffee

<table>
<thead>
<tr>
<th>Content (% db)</th>
<th>Arabica</th>
<th>Robusta</th>
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</thead>
<tbody>
<tr>
<td>Polysaccharides</td>
<td>48.5</td>
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<tr>
<td>Sucrose</td>
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<tr>
<td>Lipids</td>
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<td>12.7</td>
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<tr>
<td>Trigonelline</td>
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<td>0.7</td>
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<tr>
<td>Organic acids</td>
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<td>1.6</td>
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<tr>
<td>Proteins</td>
<td>11.3</td>
<td>12.7</td>
</tr>
<tr>
<td>Caffeine</td>
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<td>2.3</td>
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<tr>
<td>Chlorogenic acids</td>
<td>7.5</td>
<td>10.1</td>
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<tr>
<td>Ash</td>
<td>4.0</td>
<td>4.4</td>
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</table>

Nestle / Imre Blank / 12.08.2014
From the plant to the beverage - Roasting is a key step for cup quality

Species → Cultivation, harvest → Post-harvest treatment

Instant coffee technology

Instant coffee → Coffee beverage → R&G coffee
Compositional changes upon roasting define quality attributes

Sugars - Polysaccharides

Amino acids & Proteins

Lipids

Polyphenols

Aroma

Taste

Crema

Health

Colour

Nestle / Imre Blank / 12.08.2014

Nestlé Research Center

Arabinogalactan-Protein Structure

Roasting
Coffee phenols and their role in coffee aroma
Compounds formed from green coffee bean precursors upon roasting

- **Furaneol**
  - Caramelize

- **HMF**
  - Caramelize

- **Sucrose, glucose, fructose** (arabinogalactans)
  - SUGARS
  - Fragmentation
  - Maillard, Strecker

- **Nicotinic acid**
  - Pyridine and derivatives

- **Trigoneline**
  - AMINO ACIDS (Strecker-active AA)

- **Chlorogenic acid lactones**
  - CHLOROGENIC ACIDS

- **Quinic acid**
  - Quinic acid lactone
  - ORGANIC ACIDS
  - Carbonyls
  - 2-Furfurylthiol
  - 3-Mercapto-3-methyl-butyl-formate

- **E-β-Damascenone**
  - CAROTENOIDS

- **Carbonyls**

- **Caffeic + Ferulic acids**
  - Vanillin
  - Guaiacols

- **CO₂**
  - Formic, acetic, glycolic, lactic

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Chlorogenic acids as aroma precursors

Chlorogenic acid

HHQ

quinic acid

caffeic acid

ferulic acid

catechol 4-vinylcatechol 4-ethylcatechol 3,4-dihydroxybenzaldehyde
guaiacol 4-vinylguaiacol 4-ethylguaiacol vanillin
Important aroma compounds in roasted coffee

<table>
<thead>
<tr>
<th>Compound</th>
<th>Arabica</th>
<th>Robusta</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E)-beta-damasconone</td>
<td>260000</td>
<td>270000</td>
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<tr>
<td>furfurylthiol</td>
<td>110000</td>
<td>170000</td>
</tr>
<tr>
<td>MMBF</td>
<td>37000</td>
<td>33000</td>
</tr>
<tr>
<td>MBT</td>
<td>27300</td>
<td>27700</td>
</tr>
<tr>
<td>3-isobutyl-2-methoxypyrizin</td>
<td>16600</td>
<td>2400</td>
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<tr>
<td>homofuraneol</td>
<td>15000</td>
<td>12000</td>
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<td>furaneol</td>
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<td>5700</td>
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<td>2,3-butandione</td>
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<td>3190</td>
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<td>4-vinylguaiacol</td>
<td>3200</td>
<td>8900</td>
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<tr>
<td>guaiacol</td>
<td>1700</td>
<td>11000</td>
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<td>2,3-pentandione</td>
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<td>660</td>
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<td>vanillin</td>
<td>192</td>
<td>644</td>
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<td>2-ethyl-3,5-dimethylyrazin</td>
<td>165</td>
<td>470</td>
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<td>2,3-diethyl-5-methylyrazin</td>
<td>95</td>
<td>310</td>
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<td>sotolon</td>
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<tr>
<td>4-ethylguaiacol</td>
<td>32</td>
<td>362</td>
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<tr>
<td>abhexon</td>
<td>21</td>
<td>11</td>
</tr>
</tbody>
</table>

(Semmelroch et al., 1995)

Phenolic impact compounds

4-vinylguaiacol (clove-like)

Guaiacol (smokey)

Vanillin (vanilla-like)

4-ethylguaiacol (spicy, smokey)
Coffee staling has multiple origins - Degradation of sensitive aroma compounds

Blank et al. (2000, 2002)

Munro et al.
(2003)

radical induced oxidation (C-radical)

oxidation - direct or radical induced (S-radical)

reaction with aldehydes/heterocycles

nucleophilic addition at melanoidins

nucleophilic addition at chlorogenic acid derivatives

Müller & Hofmann
(2005)

Hofmann & Schieberle
(2002)

Milo et al.
(unpublished)
Influence of warm-keeping (70 °C) on the concentrations of the thiols FFT and MMBF

- No oxidation, as no corresponding disulfides were detectable!
Biomimetic in-bean experiments - Using exhausted coffee beans as reactor

Reloading exhausted coffee beans with

- nitrogen-containing compounds
  - caffeine
  - trigonelline
  - amino acids
  - amino acids + carbohydrates
- oxygen-containing compounds
  - carbohydrates
  - organic acids
  - chlorogenic acid fraction

Bean solubles

- LMW-BS
- HMW-BS

Bean solids

Exhaustive hot water extraction

Freeze-drying (48h) to 6% water, roasting, grinding, percolation

All compounds and fractions were used in natural concentrations
Decrease of free 2-furfurylthiol in coffee brew

Coffee brew made of reference beans and extracted beans

Coffee brew made of beans loaded with coffee ingredients

reference coffee bean solids
bean solids + bean solubles

reference coffee bean solids
trigonelline, amino acids, and soluble carbohydrates
quinic acid
5-caffeoylquinic acid
caffeic acid
each + transition metals

(Müller et al, 2007)
Trapping of key odorants (thiols) by polyphenols via oxidative coupling

(Müller et al, 2007)
(EP 1902628 A1)
(WO 2008/031848 A1)

Hydroxyhydroquinone (HHQ)

Carbohydrates / Amino acids

Further oxidative degradation
Coffee phenols and their role in coffee taste
Consumer liking is driven by bitterness, but not less bitterness is requested generally.

- For nearly 70%, bitterness is a liking key driver.
- 30% will not care.
- 20-25% of consumers will like 20-25% bitterness.
- ~50% like low or medium bitter coffee.
- ~15-20% like high bitter coffee.

Bitterness modulation is important.
Major bitter compounds of coffee are unknown

Approach
Reconstitute known coffee tastants in a high molecular weight tasteless fraction (>3500 Da)

Conclusion
Known compounds seem to play a minor role in coffee bitterness

* Recombinate: caffeine, trigonelline, chlorogenic acid, and quinic acid

Caffeine only contributes to about 15% to coffee bitterness
CGAs as precursors of bitter tasting lactones

- Lactone formation is well known (Farah et al., 2005)
- Lactones identified as bitter compounds in coffee (Kraehenbuehl et al. 2005, Frank et al. 2006) giving pleasant coffee-like bitter taste

<table>
<thead>
<tr>
<th>Compound</th>
<th>Bitter threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-O-caffeoyl-γ-quinide (2a)</td>
<td>13.4 40</td>
</tr>
<tr>
<td>4-O-caffeoyl-γ-quinide (3a)</td>
<td>12.1 36</td>
</tr>
<tr>
<td>5-O-caffeoyl-epi-δ-quinide (4a)</td>
<td>60.5 180</td>
</tr>
<tr>
<td>4-O-caffeoyl-muco-γ-quinide (5a)</td>
<td>11.2 30</td>
</tr>
<tr>
<td>5-O-caffeoyl-muco-γ-quinide (6a)</td>
<td>9.7 29</td>
</tr>
<tr>
<td>3-O-feruoyl-γ-quinide (2b)</td>
<td>13.7 39</td>
</tr>
<tr>
<td>4-O-feruoyl-γ-quinide (3b)</td>
<td>13.7 39</td>
</tr>
<tr>
<td>3,4-O-dicaffeoyl-γ-quinide</td>
<td>4.8 9.8</td>
</tr>
<tr>
<td>3,5-O-dicaffeoyl-epi-δ-quinide</td>
<td>24.9 50</td>
</tr>
<tr>
<td>4,5-O-dicaffeoyl-muco-γ-quinide (3a)</td>
<td>4.8 9.8</td>
</tr>
</tbody>
</table>

(Frank et al., 2006)
CGAs as precursors of tastants: Phenylindanes

- Phenylindanes another class of bitter compounds formed from CQA degradation giving a rather unpleasant harsh coffee-like bitter taste

<table>
<thead>
<tr>
<th>Compound</th>
<th>Bitter threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phenylbutanes</td>
<td>6 mg/l, 23 µmol/l</td>
</tr>
<tr>
<td>Phenylbutenes</td>
<td>39 mg/l, 145 µmol/l</td>
</tr>
<tr>
<td>Phenylindanes</td>
<td>9-40 mg/l, 32-148 µmol/l</td>
</tr>
<tr>
<td>Diphenylindanes</td>
<td>15-27 mg/l, 37-67 µmol/l</td>
</tr>
</tbody>
</table>

(Frank et al., 2007)
CGA as precursors of tastants: Furan benzene diols

- Benzene diols are formed from catechols and furan derivatives having unpleasant harsh bitter taste (Kreppenhofer et al. 2010)

\[
\text{furfuryl alcohol} \quad \xrightarrow{\text{H}^+ - \text{H}_2\text{O}} \quad \text{catechol} \quad + \quad 4-(\text{furan-2-ylmethyl})\text{benzene-1,2-diol}
\]
Formation of bitter tastants upon roasting

- Bitter precursor content depends on blend
- Bitter compound formation depends on roasting degree
- Kinetics are different for different chemical classes
- Bitter quality is also different

<table>
<thead>
<tr>
<th>Compound class</th>
<th>Threshold for bitterness (μmol/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Caffeine</td>
<td>750</td>
</tr>
<tr>
<td>Lactones</td>
<td>30-200</td>
</tr>
<tr>
<td>DKPs</td>
<td>190-4000</td>
</tr>
<tr>
<td>Phenylindanes</td>
<td>30-150</td>
</tr>
<tr>
<td>Benzenediols</td>
<td>50-800</td>
</tr>
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</table>

Diketopiperazines (DKPs)
Coffee phenols and their role in coffee crema
Activity guided approach applied to studying coffee crema

- Measuring foamability & foam stability: using Fometube, Ultraturrax foamer

- Activity guided separation: soluble fraction / precipitate, LMW / HMW (using ammonium sulfate and isopropanol)

- Isolation: Preparative foam fractionation

- Identification: NMR, HPLC-MS

- Model experiments: Roasting (polyphenols, polysaccharides)

- Addition of foaming fractions to coffee (evaluating foamability & foam stability)
Influence of roasted caffeic acid (rCA) on foamability/stability

Test in instant espresso powder (1g/100 mL)

(Ultraturrax)

(Kornas et al, unpublished)
Formation of foaming compounds in coffee by 4-vinylcatechol oligomerization

(Kornas et al, unpublished)
New foaming compounds identified in coffee crema (espresso)

4-Vinylcatechol oligomers

(EP 12199583.1)  (WO 2014102229 A1)

Quinic acid esters

Fatty acid sucrose esters

(Kornas et al, unpublished)
Foam structure of espresso spiked with foam enhancers

Espresso + 0.5% FASE
Espresso + 0.007% roasted CA

(Kornas et al, unpublished)
Foam structure of espresso spiked with different foam enhancers (Foamscan)

- Espresso 0.5%
- Espresso 0.5% + Sucr.-pal. 0.05%
- Espresso 0.5% + roasted CA 0.007%

(Kornas et al, unpublished)
Coffee crema - Summary

Activity-guided fractionation of espresso crema revealed 3 groups of foam enhancing molecules:

- **Fatty acid sucrose esters:** already present in the raw bean, being degraded upon roasting
- **Quinic acid esters & quinides:** formed upon thermal transesterification of quinic acid
- **4-Vinylcatechol oligomers:** formed upon thermal degradation of caffeic acid and chlorogenic acid

Similar foam activity can be achieved by sucrose stearate (0.5%), quinoyl palmitate (0.025%), and 4-vinylcatechol oligomers (0.007%), but the resulting foam structure is different:

- Sucrose esters and quinic acid ester decrease surface tension and viscoelasticity and generate a **dry, course foam**
- 4-Vinylcatechol oligomers do not affect surface tension, but increase viscoelasticity and generate a **fine crema-like foam**
Conclusions:
The role of polyphenols in coffee quality

• Chlorogenic acids play a crucial role in the formation and degradation of important coffee aroma compounds

• Chlorogenic acids are the main precursors of several bitter tasting compounds in coffee

• Chlorogenic acids degradation products contribute to the crema of coffee

• Knowing the chemical structure of key compounds allow using them as quality markers

• In addition, coffee polyphenols play an important role as health promoting substances
The key to success

- Profound base in chemistry
- Inventive approach in experimentation
- Working at the interface of scientific disciplines
- Addressing complex phenomena, challenging the status-quo
- Multidisciplinary approach, with chemistry gluing all together
- Continuous learning capacity & creativity
- Open to share and ready to collaborate
But one thing is sure ...

... Coffee is the most pleasurable hot beverage in the world
Coffee phenols and their role for health
The importance of coffee polyphenols in human diet

<table>
<thead>
<tr>
<th>Food</th>
<th>Food group</th>
<th>Serving (g)</th>
<th>Polyphenols</th>
<th>Polyphenols A%</th>
<th>Antioxidants</th>
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<td>1</td>
<td>115</td>
<td>1</td>
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<td>Black bean</td>
<td>Seeds</td>
<td>35</td>
<td>40</td>
<td>52</td>
<td>1216</td>
</tr>
</tbody>
</table>

Coffee

- 36. place in mg/100g
- 6. place per serving
- 1. place for daily consumption (3-4 cups per day)

(Scalbert et al, 2010)
CQAs most contributors to polyphenol intake in French adults

Dietary intake of 337 polyphenols in French adults

Jara Pérez-Jiménez, Léopold Feuzeu, Mathilde Touvier, Nathalie Arnault, Claudine Manach, Serge Hercberg, Pilar Galan, and Augustin Scalbert

AJCN, 2011

SU.VI.MAX cohort
4,942 men & women
24-hr dietary records (x6)

Flavanones

Flavonols

Anthocyanins

Catechins

Proanthocyanidins

Hydroxybenzoic acids

Hydroxycinnamic acids

203 mg/day
271 mg/day
198 mg/day

36 mg/day
32 mg/day
31 mg/day

1.19 g/day

The most complete data on polyphenol intake

337 polyphenols consumed by French adults

(Scalbert et al, 2011)
More and more reports on positive effects on health for a moderate coffee consumption

- Robust inverse relation between regular coffee consumption, including decaffeinated, and risk of type 2 diabetes based on meta-analyses of epidemiological studies (van Dam 2006; van Dam and Hu 2005)
- Coffee, decaffeinated coffee, and tea consumption in relation to incident type 2 diabetes mellitus: a systematic review with meta-analysis. (Huxley et al 2009)
- The use of green coffee extract as a weight loss supplement: a systematic review and meta-analysis of randomised clinical trials. (Onakpoya et al 2011)
- Lipophilic antioxidants more neuroprotective than hydrophilic (e.g. lactones (Chu et al 2009)
- High CQA coffees prevent oxidative damage (Hoelzl et al 2010)
- Antioxidant rich coffee reduces DNA damage (Bakuradze et al, 2011)
- CGA rich coffee induce chemopreventive phase II enzymes (Boettler et al. 2011)
- Coffee has positive effects to reduce cognitive decline (Abreu et al, 2011)
- N-Methylpyridinium stimulates respiratory activity and promotes glucose utilization in HepG2 cells (Riedel et al., 2014)
Antioxidant activity of green and roasted coffee

80% of the total antioxidant activity in green coffee comes from the 9 main chlorogenic acid

Antioxidant activity in roasted coffee stays at high level but is less explained by CGAs

(Leloup et al, ASIC 2010)
Antioxidant activity of roasted coffee derives mainly from an unresolved hump
Precursor ion scan by LC/MS of a roasted coffee to detect precursors of caffeic acid moiety

Caffeic acid moiety largely present in unresolved hump

Leloup et al, ASIC 2010
Model roasting of 5-CQA at 200°C in dry state

Degradation of 5-CQA and Folin of reaction mixture

HPLC chromatogram from final reaction mixture

- 5-CQA is rapidly degraded in model roast mix at 200°C
- TPP by Folin of reaction mixture remains almost constant
- Lactones are formed but cannot explain loss of 5-CQA and Folin values
- A lot of minor peaks are detectable
Direct infusion into LC/MS of model roast of 5-CQA Polymerization of CQA can be observed

DiCQA
Di-CQL

CQA
CQL

+174 QA-H2O

+162 CA-H2O

+162 CA-H2O

+174 QA-H2O

+174 QA-H2O

polymers
Possible transformations of CGA and the effect on AOX properties

Chlorogenic acid
Polymerization
Transformation
Degradation

AOX property

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