



Nestlé Research™



ADVANCED ANALYTICAL SENSORY CORRELATION – TOWARDS A BETTER MOLECULAR UNDERSTANDING OF COFFEE FLAVOUR

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Can we predict in-cup sensory profiles by analytical data?



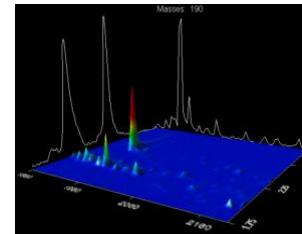
01 THE CHALLENGE

SENSORY – ANALYTICAL CORRELATION
STATE OF THE ART



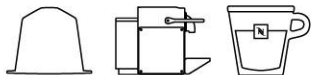
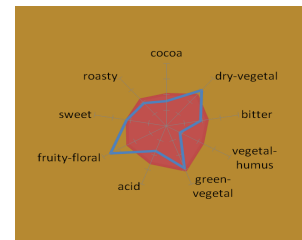
02 THE APPROACH

MONADIC SENSORY PROFILING
TARGETED GC/MS ANALYSIS
ADVANCED STATISTICS



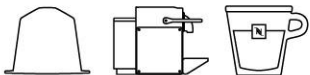
03 THE SOLUTION

RELIABLE PREDICTIVE TOOL

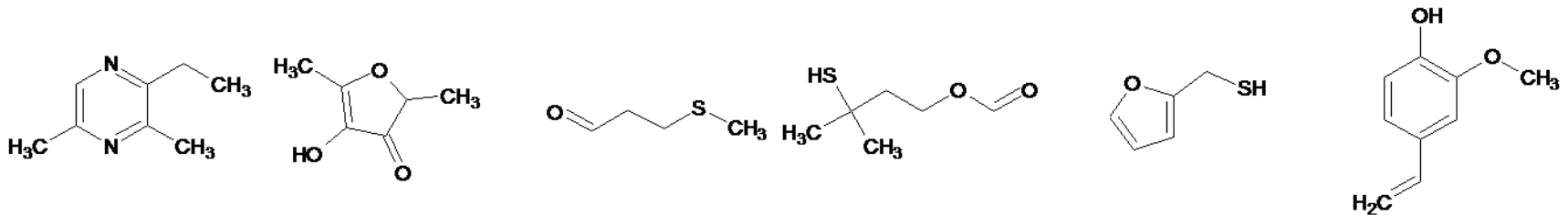
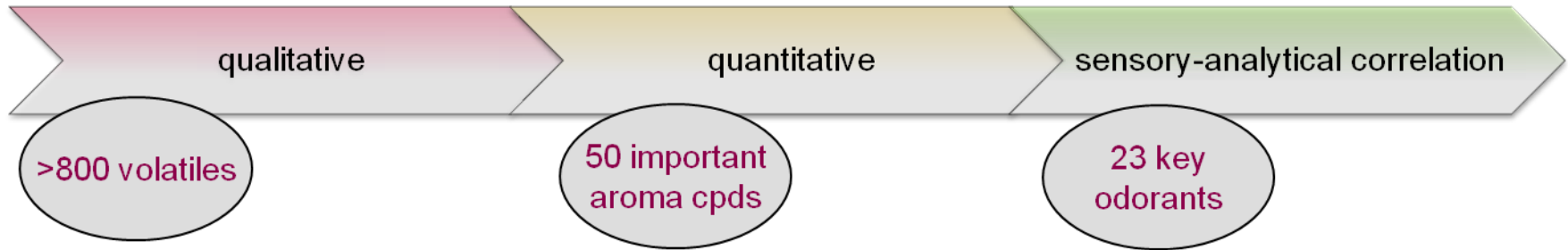


01 THE CHALLENGE

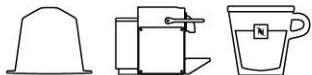
SENSORY – ANALYTICAL CORRELATION



Aroma Value Concept: a comprehensive approach to evaluate coffee aroma



Grosch W. (2001) *Chem. Senses* 26, 533-546



The coffee 'melodie' – fundamentally different nature of sensory & analytical data

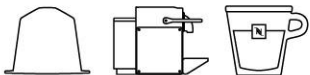
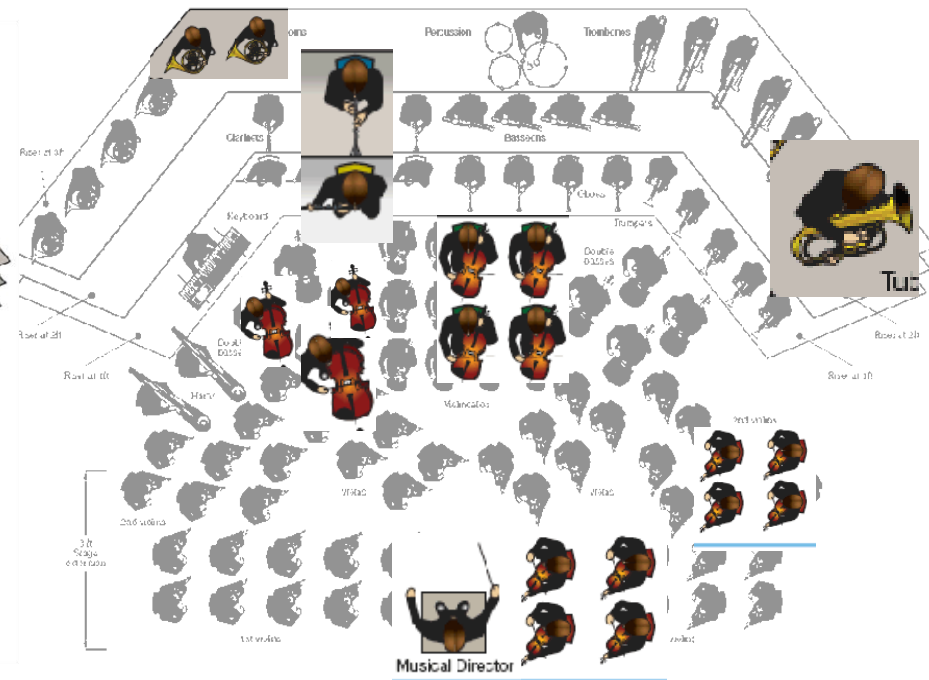
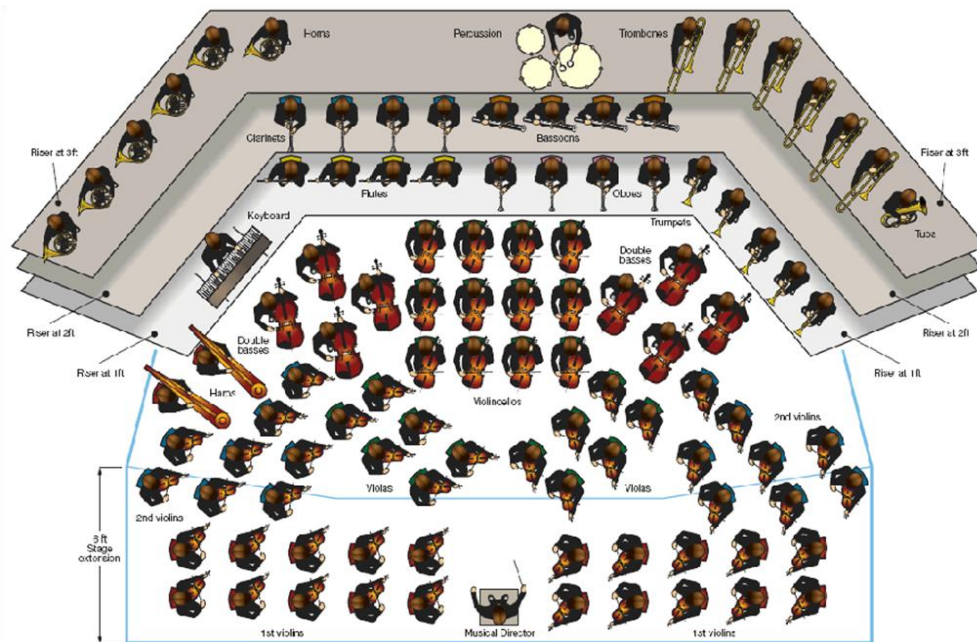


SENSORY PROFILING

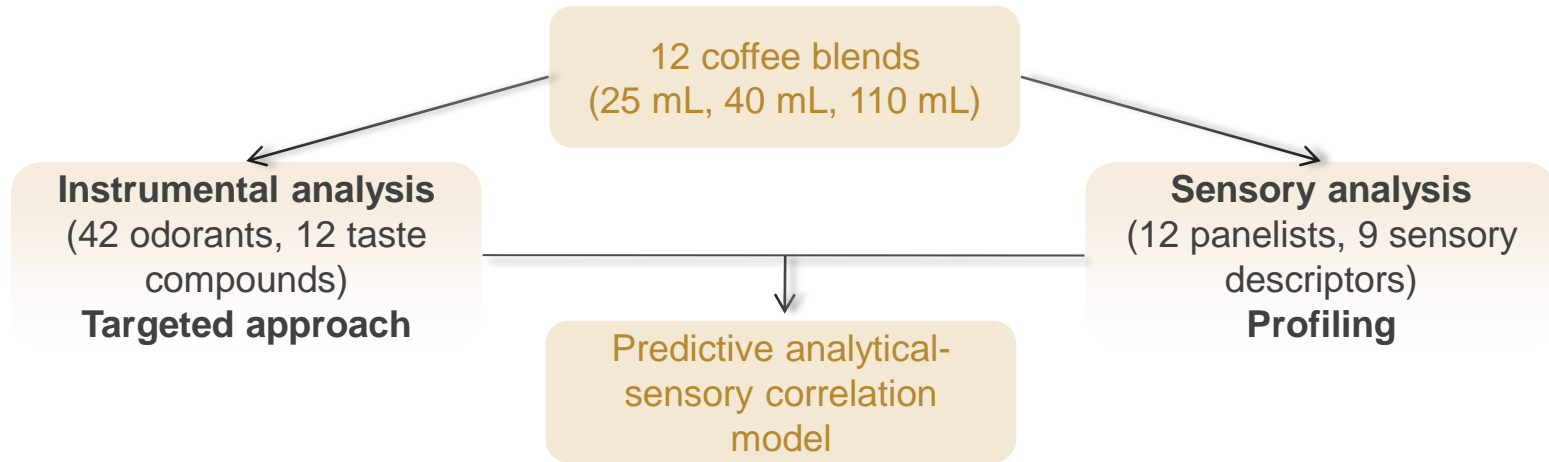
- Listen to the orchestra
- Describe specific instruments/tonalities
- Evaluate their intensities

AROMA ANALYTICS (targeted)

- Identification of the key players/instruments
- Evaluation of their concentrations & impact
- Reconstitute melodie

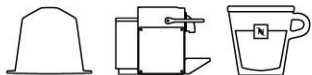


Outline & Objectives of study



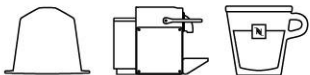
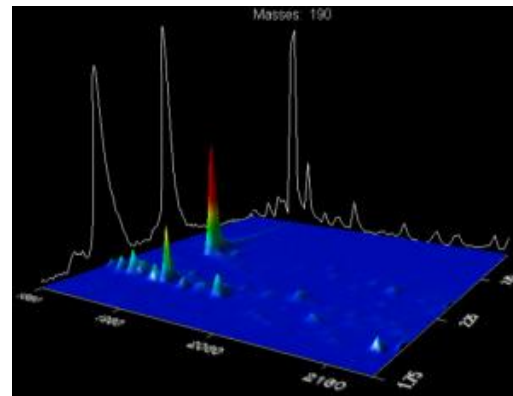
OBJECTIVES

- Develop mathematical model to predict coffee in-cup sensory profiles
- Identify well correlated marker compounds for sensory descriptors



02 THE APPROACH

MONADIC SENSORY PROFILING
TARGETED GC/MS ANALYSIS
ADVANCED STATISTICS



Sensory profiling was carried out with an expert panel (n=12)



THE BASIC ATTRIBUTES...

- roasty
- bitter
- acid

... describe the basic properties of an Espresso coffee

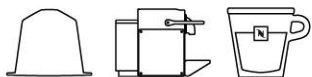
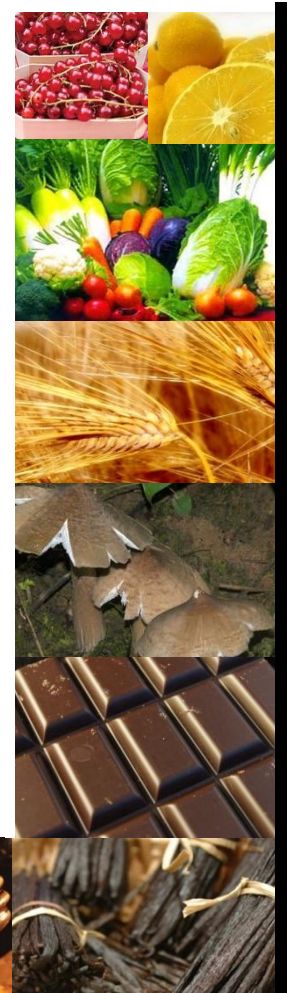


The ,subtle' aroma descriptors...

- **fruity-floral**
red fruits, lemon, jasmine
- **green-vegetal**
herbs, fresh vegetables
- **dry-vegetal**
wood, malt, cereal
- **vegetal-humus**
earthy, mushroom
- **cocoa**
roasted, cacao, dark chocolate
- **sweet**
vanilla, caramel, honey

... describe the signature aroma of an Espresso coffee

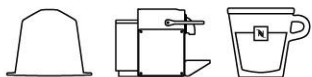
... are grouped based on olfactive similarity



In-cup concentrations of 54 aroma and taste compounds were determined



substance	flavor quality	substance	flavor quality
1 methanethiol	sulfur, garlic	28 2-acetylthiazole	roasty, popcorn
2 dimethyl sulfide	cabbage, sulfur	29 furfural	grass, almond
3 dimethyl trisulfide	sulfur, cabbage	30 furfuryl acetate	-
4 furfurylthiol	sulfur, roast	31 2,3,5-trimethylpyrazine	roasty
5 3-mercapto-3-methylbutylformate	catty	32 2-ethyl-3,6-dimethylpyrazine	roasty, earthy
6 methional	potato	33 2-ethyl-3,5-dimethylpyrazine	roasty, earthy
7 3-methyl-2-butenethiol	sulfur, amine	34 2-ethenyl-3,5-dimethylpyrazine	roasty, earthy
8 2-methyl-3-furanthiol	meat	35 2,3-diethyl-5-methylpyrazine	roasty, earthy
9 acetaldehyde	pungent, fruity	36 2-acetylpyrazine	roasty
10 propanal	solvent, pungent, fruity	37 2-isopropyl-3-methoxypyrazine	pea, earthy
11 2-methylpropanal	fruity, pungent	38 2-isobutyl-3-methoxypyrazine	pea, earthy
12 2-methylbutanal	fruity, cocoa	39 β -damascenone	rose, honey
13 3-methylbutanal	malty	40 sotolon	maggi, curry
14 phenylacetaldehyde	honey	41 furaneol	caramel
15 hexanal	grass	42 maltol	caramel
16 2,3-butanedione	buttery	43 3-CQA	-
17 2,3-pentanedione	buttery	44 5-CQA	-
18 vanilline	vanilla	45 4-CQA	-
19 ethyl 2-methylbutanoate	fruity	46 5-CQL	bitter
20 ethyl 3-methylbutanoate	fruity	47 4-CQL	bitter
21 p-cresol	medicinal, phenolic, smoke	48 5-FQA	-
22 guaiacol	smoke, medicine	49 4-FQA	-
23 4-ethylguaiacol	spice, clove	50 cyclo-Val-Pro	bitter
24 4-vinylguaiacol	spice, clove	51 cyclo-Ala-Pro	bitter
25 N-methylpyrrole	-	52 cyclo-Pro-Leu	bitter
26 pyridine	-	53 cyclo-Phe-Pro	bitter
27 2-acetylpyridine	popcorn	54 caffeine	bitter



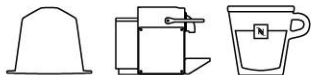
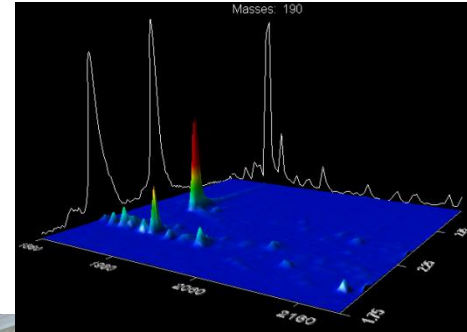
In-cup quantification was carried out using state-of-the-art methods



ABSOLUTE QUANTITATIVE DATA

- 42 aroma compounds (isotope dilution assay)
 - a. SPME-GC-MS
 - b. SPME-GCxGC-TOF MS
 - c. SPE-GC-MS

- 12 taste compounds (external standardisation)
 - a. HPLC-DAD
 - b. LC-MS/MS

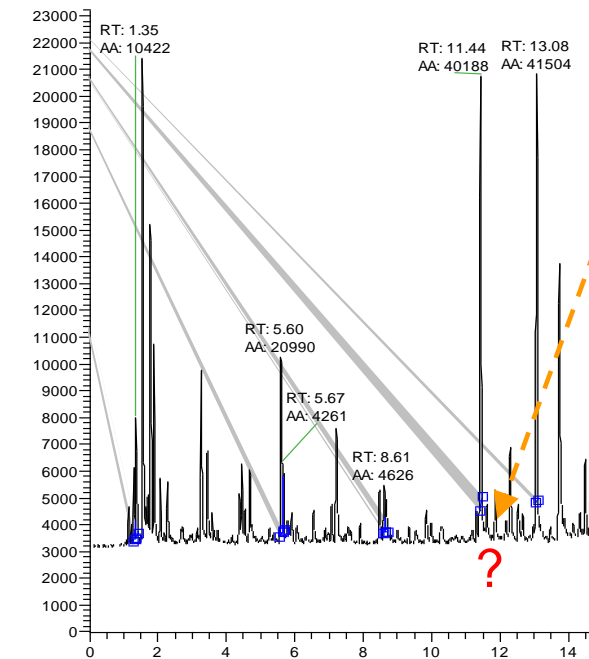


Comprehensive GCxGC-TOF MS to quantify high impact trace odorants

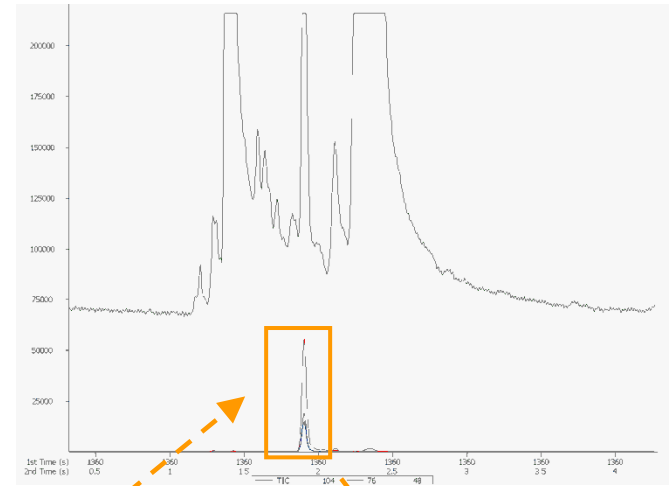


Analysis of methional

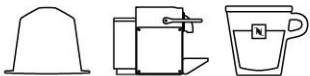
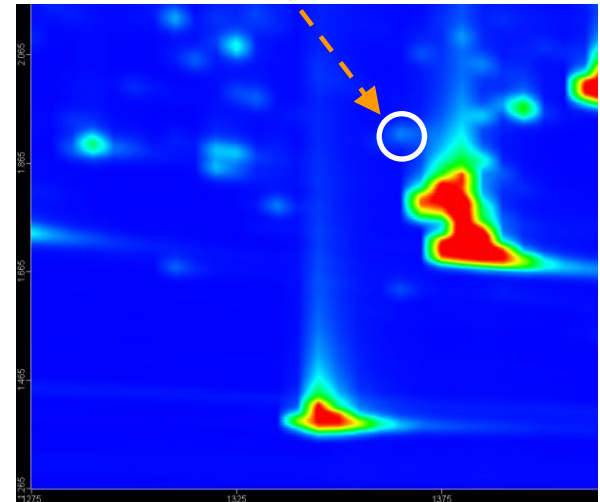
RT: 0.00 - 33.66



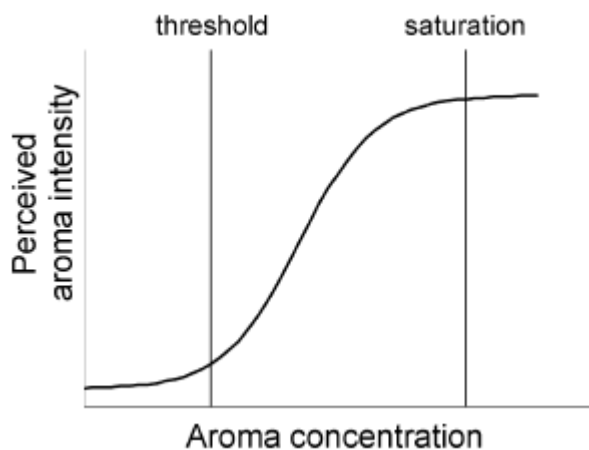
Methional peak hidden behind other peaks



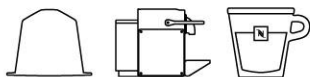
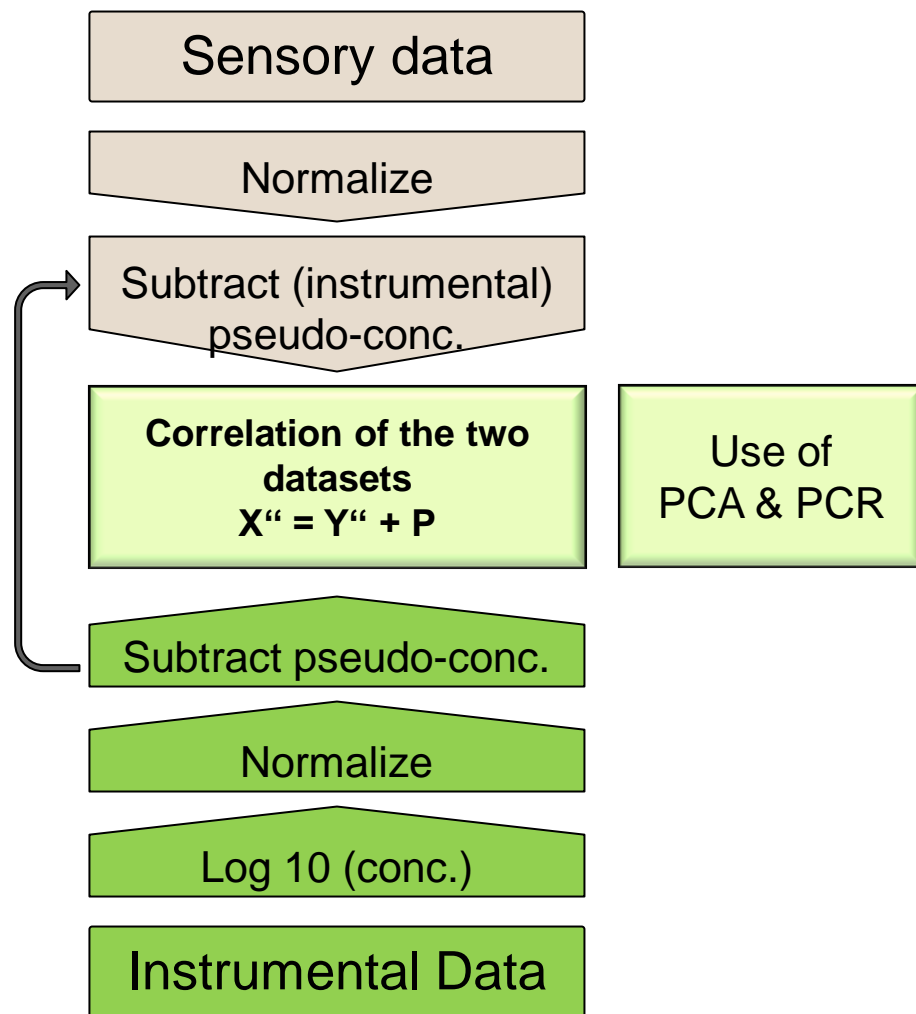
Resolved by deconvolution and 2-dimensional techniques



Preprocessing of analytical & sensory data key to perform multivariate statistics



Fechner's law:
perception $\sim k \log(\text{concentration})$



Normalisation & transformation of analytical data



Log 10 (conc.)

	methanethiol	dimethyl sulfide	dimethyl trisulfide	furfurylthiol	3-mercapto-3-methylbutylformate	acetaldehyde	propanal	2-methylpropanal	2-methylbutanal	3-methylbutanal
R1	2.67	1.92	0.42	2.24	1.32	3.73	3.36	3.50	3.48	3.39
E1	2.56	1.80	-0.11	2.10	1.10	3.49	3.14	3.36	3.25	3.13
E5	2.64	1.63	0.11	2.08	1.35	3.62	3.18	3.41	3.30	3.21
L1	2.20	1.64	-0.13	1.66	0.73	3.38	2.95	3.12	3.07	2.97
L2	2.25	1.41	0.13	1.85	0.97	3.31	3.05	3.28	3.11	2.99
R2	2.92	1.79	0.39	2.27	1.23	3.77	3.42	3.61	3.53	3.41
R3	2.88	1.63	0.30	2.24	1.33	3.66	3.35	3.70	3.43	3.31
E4	2.66	1.81	0.21	2.14	1.20	3.56	3.19	3.41	3.38	3.28
E2	2.90	2.40	0.11	2.13	1.56	3.68	3.27	3.46	3.40	3.34
E6	2.65	2.08	0.22	1.84	1.39	3.47	3.16	3.52	3.44	3.27
L3	2.17	1.56	0.08	1.85	1.14	3.28	2.95	3.19	3.08	3.01
E3	2.45	1.69	0.06	2.01	0.91	3.57	3.11	3.29	3.21	3.11
Mean	2.60	1.83	0.18	2.03	1.22	3.55	3.17	3.42	3.28	3.18
SD	0.28	0.28	0.17	0.18	0.23	0.15	0.14	0.16	0.16	0.15

Pseudo-concentration

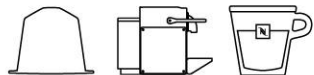
	methanethiol	dimethyl sulfide	dimethyl trisulfide	furfurylthiol	3-mercapto-3-methylbutylformate	acetaldehyde	propanal	2-methylpropanal	2-methylbutanal	3-methylbutanal	Pseudo-conc.
R1	0.31	0.29	1.40	1.18	0.43	1.20	1.32	0.54	1.23	1.35	0.95
E1	-0.17	-0.13	-1.63	0.42	-0.50	-0.42	-0.21	-0.35	-0.23	-1.34	-0.25
E5	0.18	-0.72	-0.41	0.28	0.57	0.45	0.06	-0.05	0.08	0.20	0.22
L1	-1.60	-0.68	-1.78	-2.03	-2.12	-1.15	-1.59	-1.87	-1.37	-1.43	-1.53
L2	-1.39	-1.54	-0.26	-0.98	-1.05	-1.62	-0.86	-0.84	-1.12	-1.25	-0.76
R2	1.29	-0.17	1.23	1.38	0.04	1.44	1.75	1.21	1.57	1.52	1.14
R3	1.15	-0.72	0.71	1.19	0.46	0.70	1.26	1.79	0.93	0.85	0.91
E4	0.24	-0.10	0.18	0.64	-0.08	0.04	0.16	-0.03	0.60	0.65	0.21
E2	1.21	2.02	-0.40	0.59	1.44	0.88	0.69	0.24	0.69	1.01	0.24
E6	0.20	0.89	0.25	-1.05	0.72	-0.53	-0.10	0.62	0.99	0.54	0.13
L3	-1.74	-0.99	-0.56	-0.97	-0.35	-1.82	-1.53	-1.44	-1.28	-1.16	-1.09
E3	-0.60	-0.52	-0.67	-0.10	-1.31	0.10	-0.44	-0.80	-0.48	-0.47	-0.18

Pseudo-composition

	methanethiol	dimethyl sulfide	dimethyl trisulfide	furfurylthiol	3-mercapto-3-methylbutylformate	acetaldehyde	propanal	2-methylpropanal	2-methylbutanal	3-methylbutanal
R1	-0.64	-0.65	0.46	0.23	-0.51	0.26	0.37	-0.41	0.28	0.40
E1	0.08	0.13	-1.38	0.67	-0.25	-0.17	0.04	-0.10	0.02	-0.09
E5	-0.04	-0.94	-0.63	0.06	0.35	0.23	-0.16	-0.27	-0.14	-0.02
L1	-0.07	0.85	-0.25	-0.50	-0.59	0.38	-0.06	-0.34	0.16	0.10
L2	-0.63	-0.77	0.50	-0.22	-0.29	-0.86	-0.09	-0.07	-0.36	-0.48
R2	0.15	-1.31	0.09	0.24	-1.10	0.30	0.61	0.07	0.43	0.38
R3	0.24	-1.64	-0.20	0.27	-0.46	-0.21	0.34	0.88	0.02	-0.06
E4	0.03	-0.31	-0.04	0.43	-0.29	-0.17	-0.06	-0.24	0.39	0.43
E2	0.97	1.79	-0.63	0.35	1.20	0.64	0.45	0.00	0.46	0.77
E6	0.07	0.76	0.12	-1.17	0.59	-0.66	-0.22	0.49	0.86	0.42
L3	-0.65	0.10	0.53	0.12	0.74	-0.73	-0.44	-0.35	-0.19	-0.08
E3	-0.42	-0.34	-0.49	0.08	-1.13	0.28	-0.26	-0.62	-0.30	-0.29

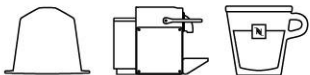
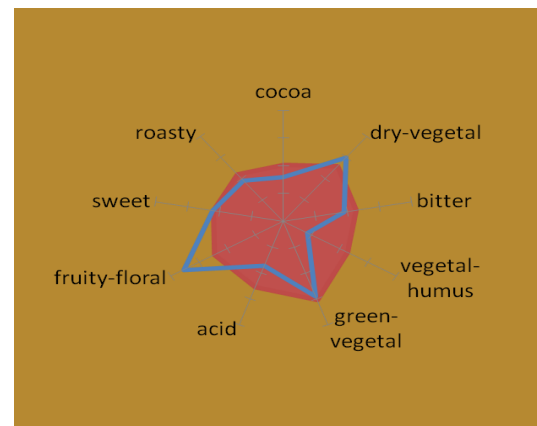
Standardize 'weight' of each compound across coffees
 $Y1 = (X1 - \text{mean}) / \text{SD}$

Subtract pseudo-concentration as per coffee
 $Y2 = Y1 - \text{mean conc.}$

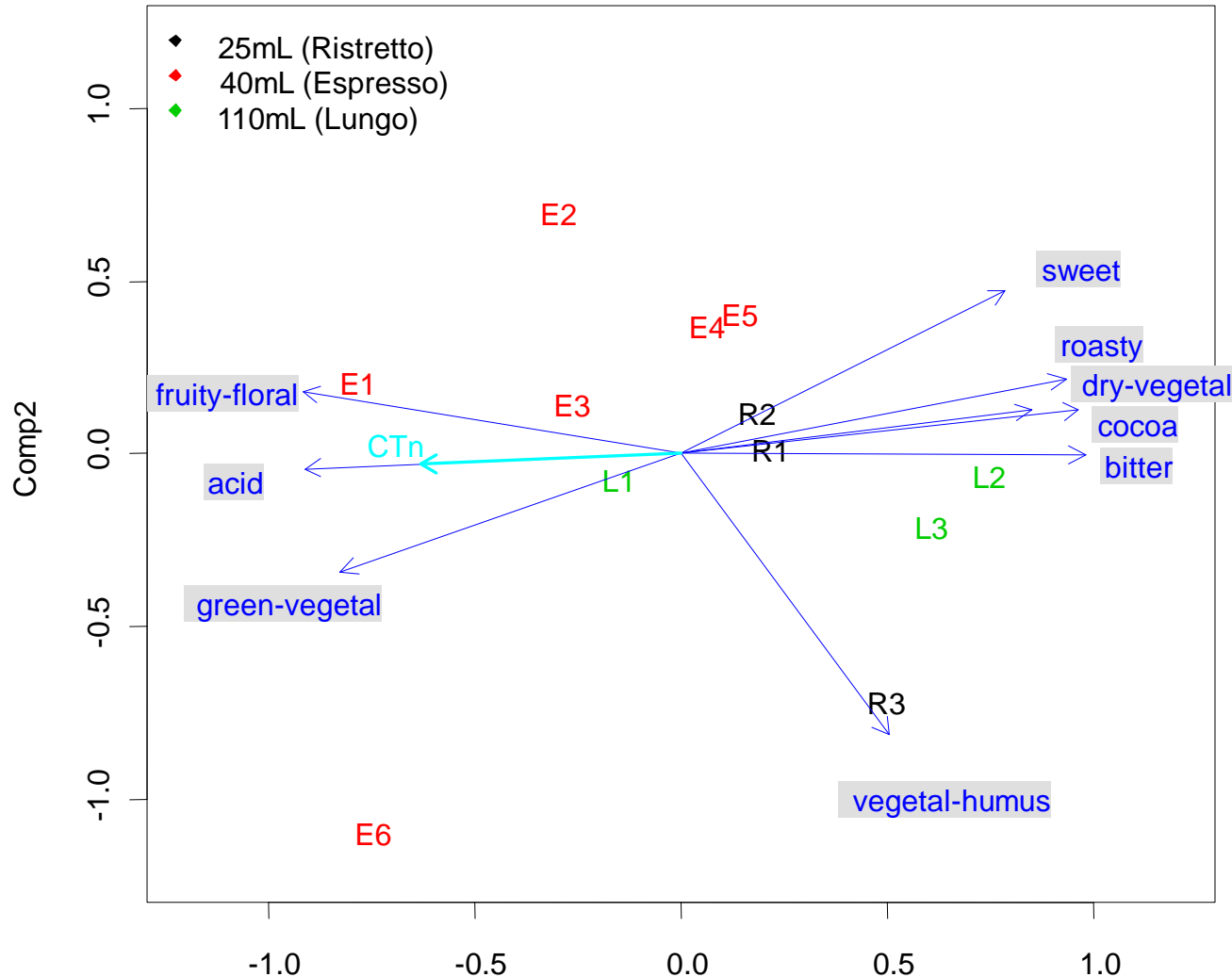
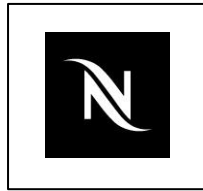


03 THE SOLUTION

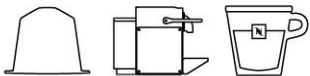
RELIABLE PREDICTIVE TOOL
FOR IN-CUP SENSORY PROFILES



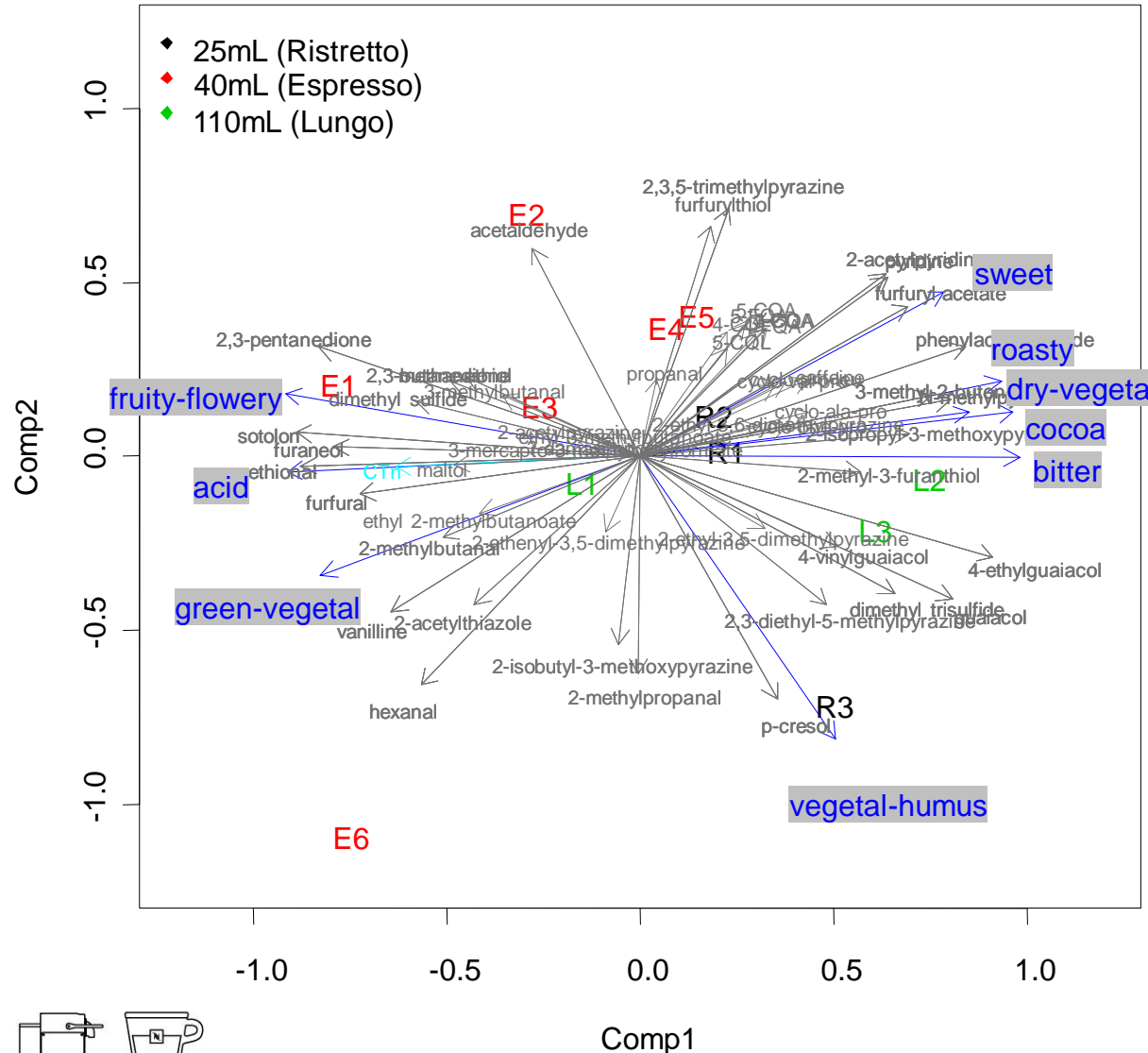
Coffees are widely distributed over sensory space



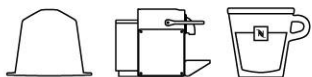
PCA from Sensory data
(subtracted 'intensity effect')



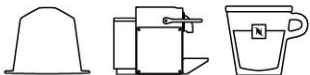
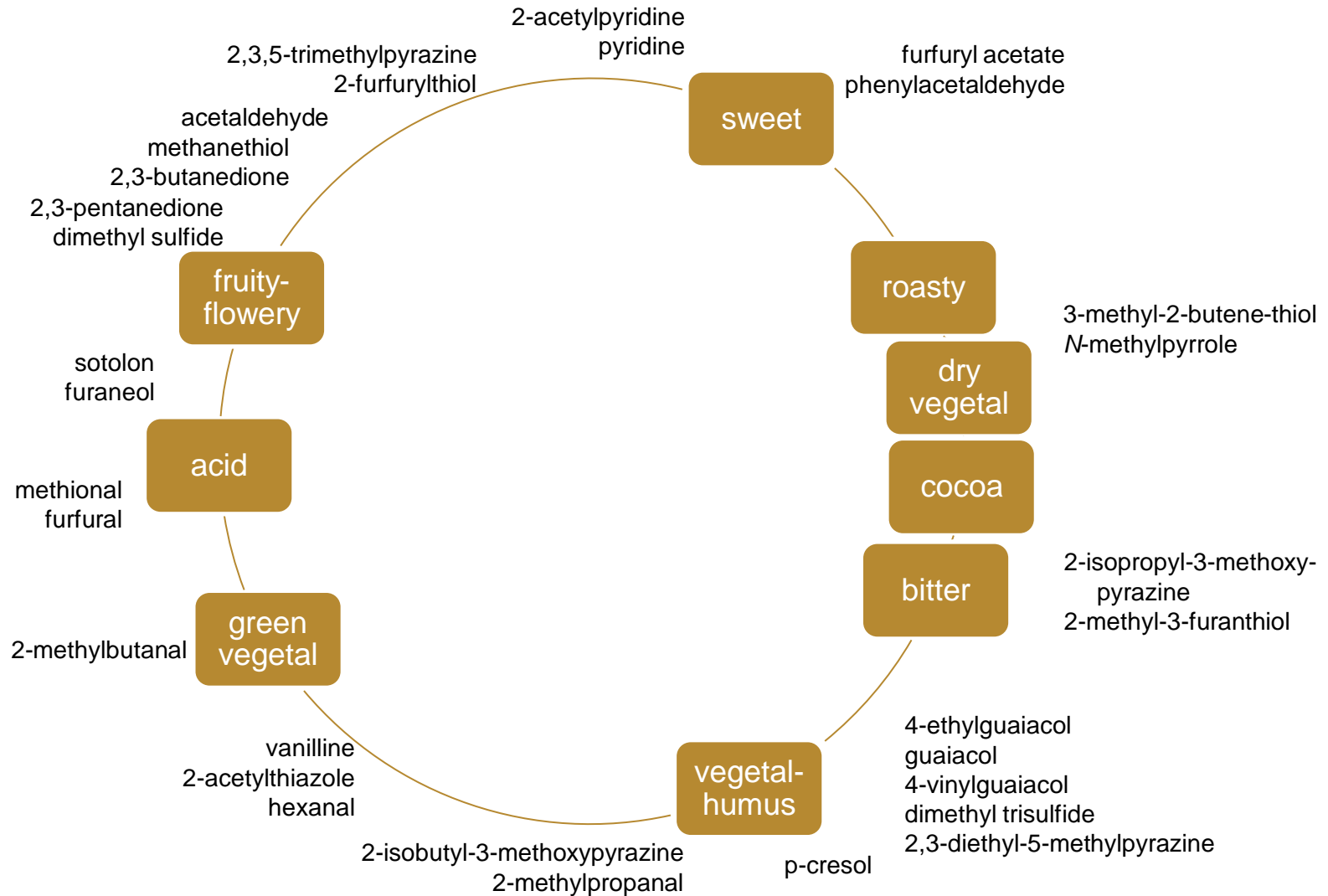
Combination of sensory & analytical spaces using PCA



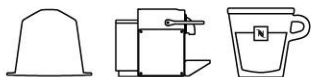
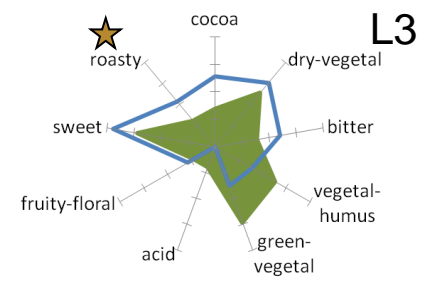
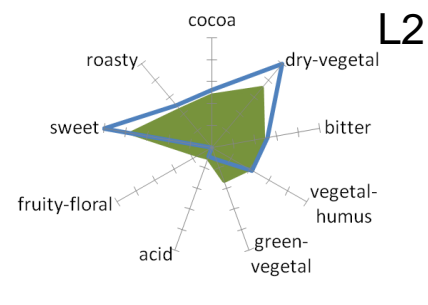
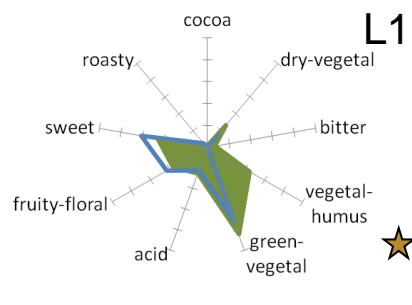
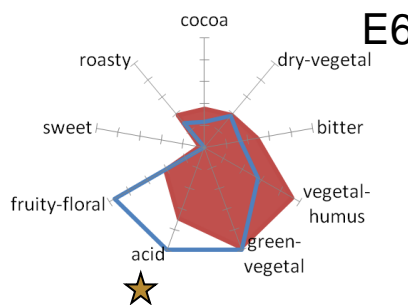
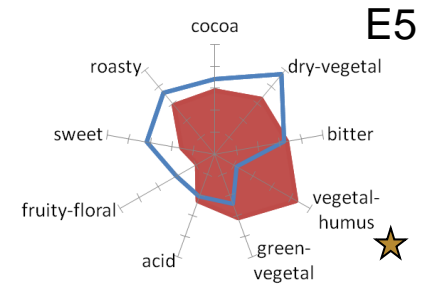
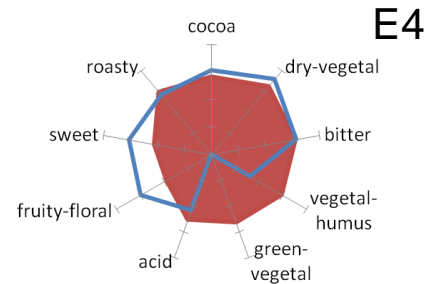
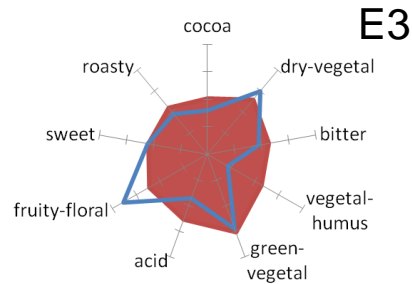
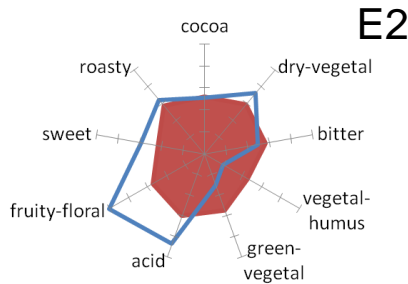
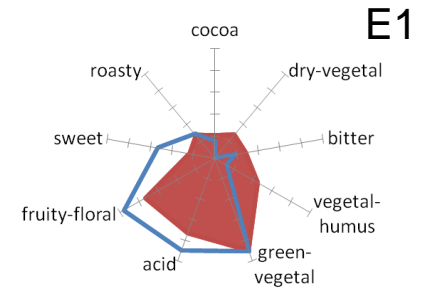
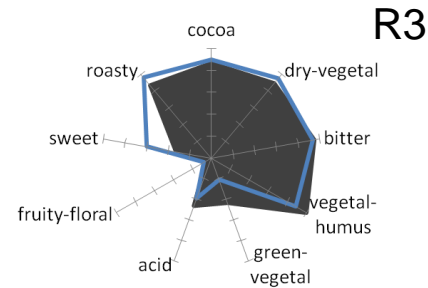
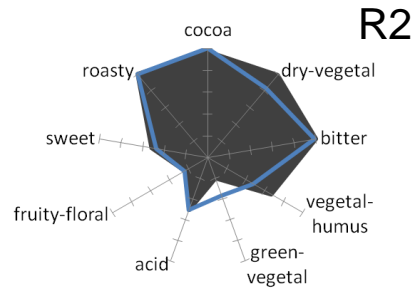
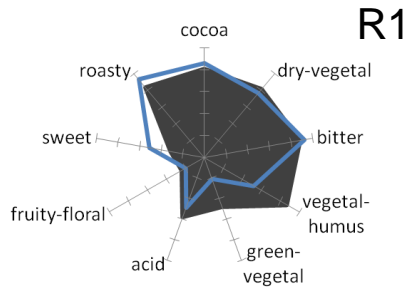
- Correlated arrows are close to each other
- The longer an arrow, the better its representation in sensory space



30 compounds exhibit strong correlation to the sensory descriptors



The robust statistical model allows a reliable prediction of the sensory profile, i.e. 101 out of 106 data are below LSD



CONCLUSIONS

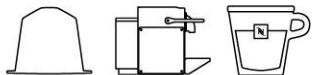


- A mathematical model has been developed which allows predicting the sensory in-cup profiles of Nespresso blends
- Deeper understanding of link between sensory descriptors and aroma markers
- Useful tool to support development of Nespresso blends with new taste experiences

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■ Deeper understanding of link between sensory descriptors and aroma markers

■ Useful tool to support development of Nespresso blends with new taste experiences



Thank you for your
attention!



ANY QUESTIONS ?



Nestlé Research™