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Bath, United Kingdom

Founded in 3





The Roman Baths

Boston, Massachusetts

Founded in 1630





Eugene, Oregon

Founded in 1846



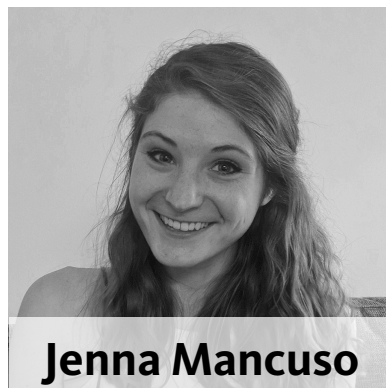


Hendon Materials Simulation



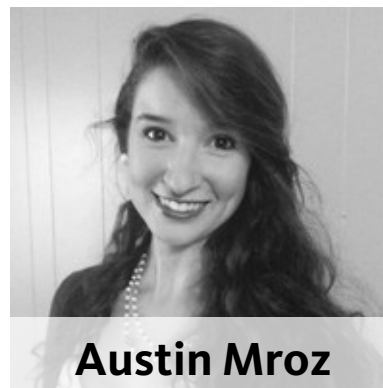
Tom W. Kasel

Photovoltaics, defects,
semiconductors



Jenna Mancuso

MOFs, wine,
reaction mechanisms



Austin Mroz

Cheminformatics, MOFs,
materials discovery



Lya Carini

Organic solvation,
molecular redox



Chase Callahan

Transition metal carbides,
core@shell catalysts



Jack Yang

Molecular redox,
crystal formation

Coffee projects

UO coffee lab
Coming 2019

2019 students

Porous conductors,
software development

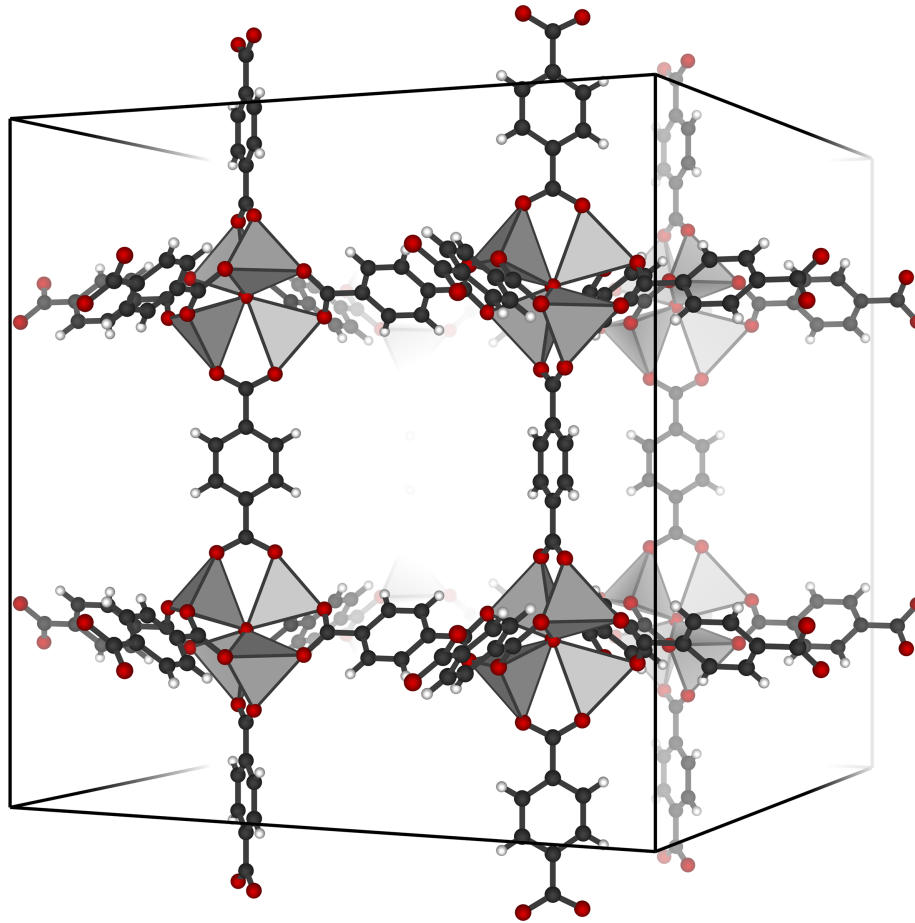
Rotation Students

Andy Swansiger



Metal-organic frameworks

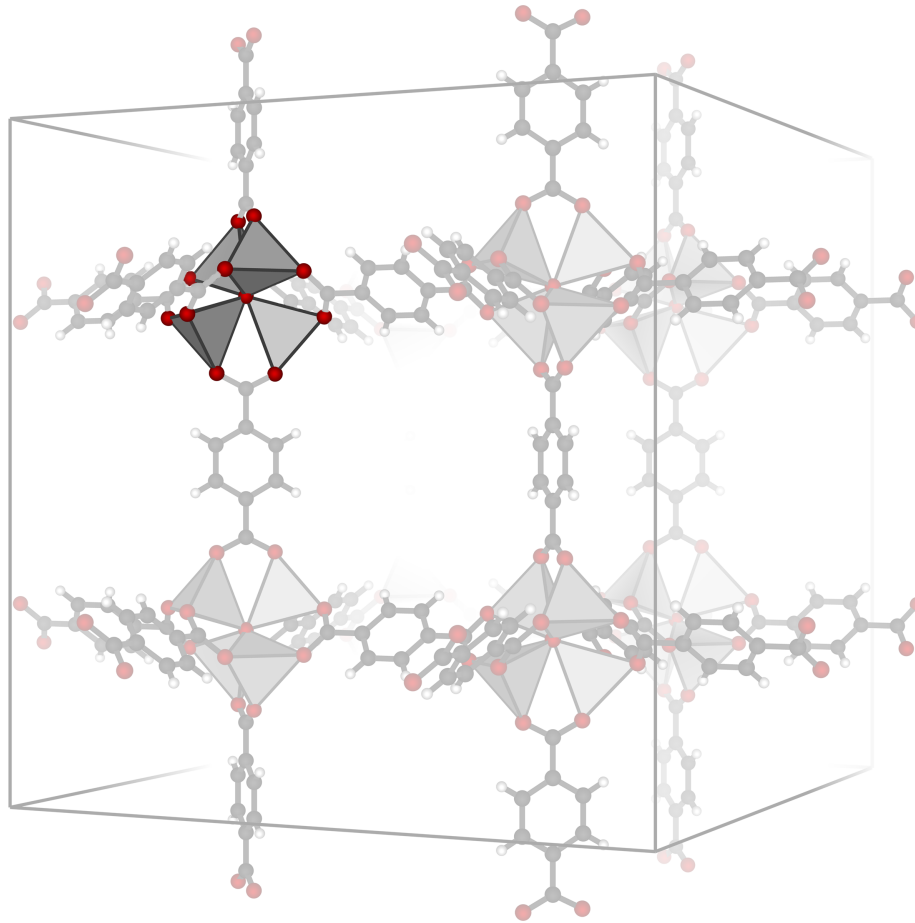
A class of porous materials for energy storage and conversion





Metal-organic frameworks

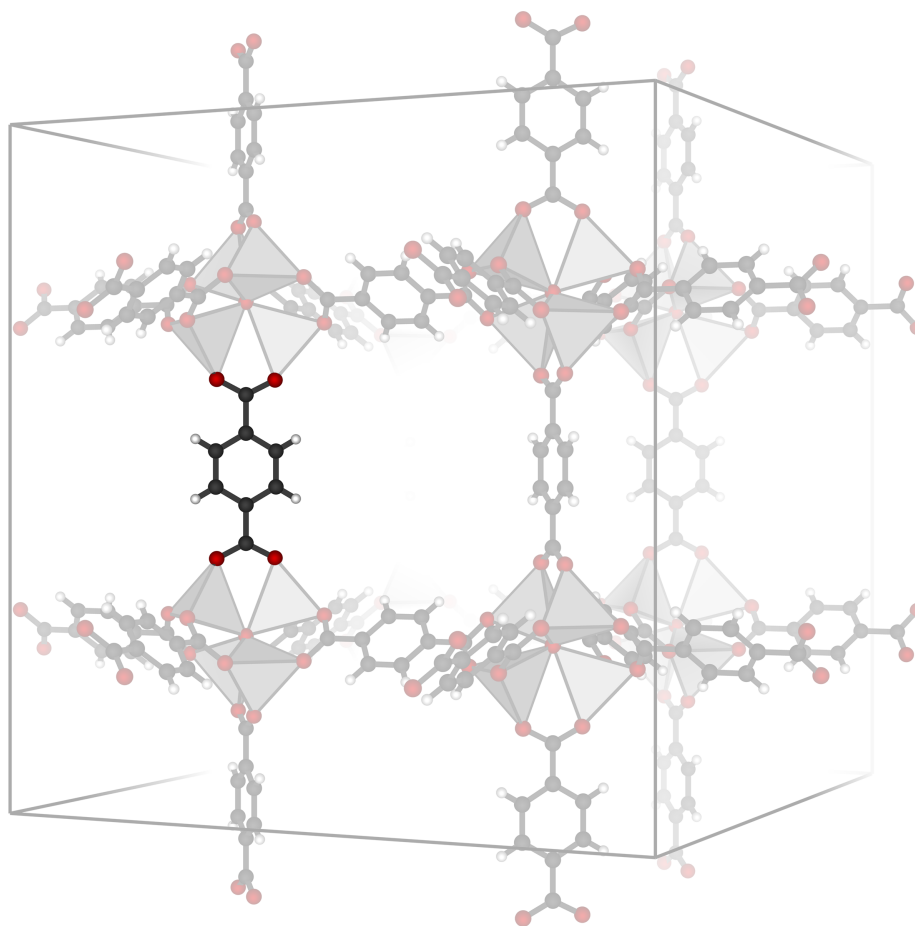
MOFs contain metal-clusters



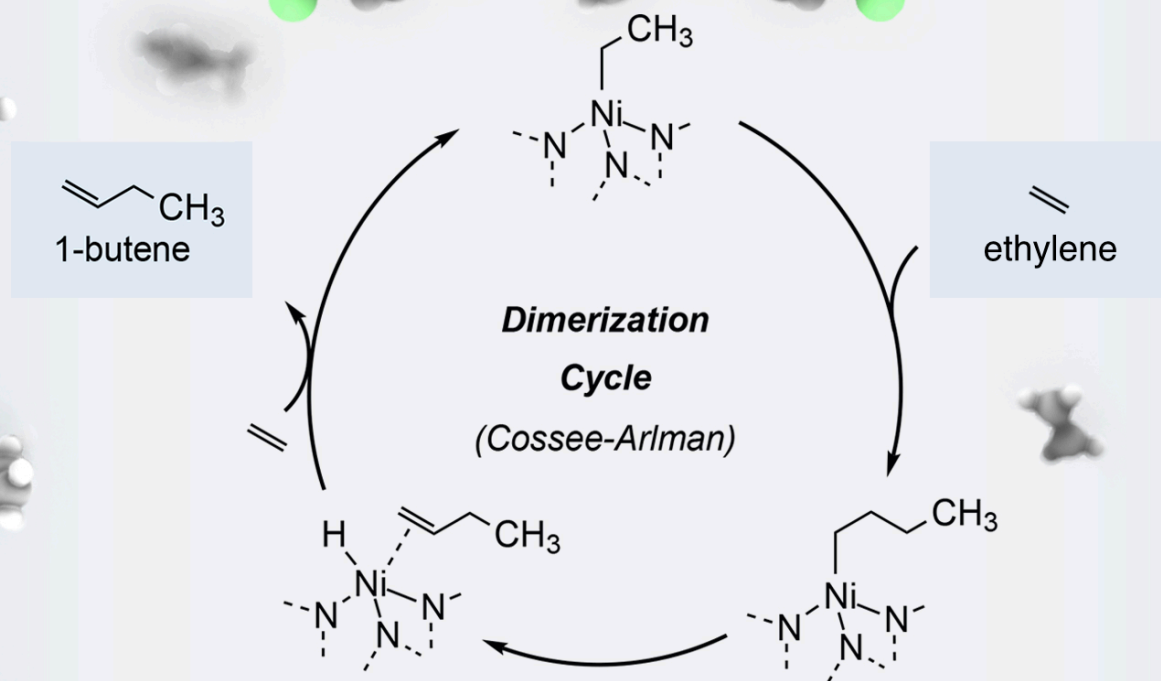


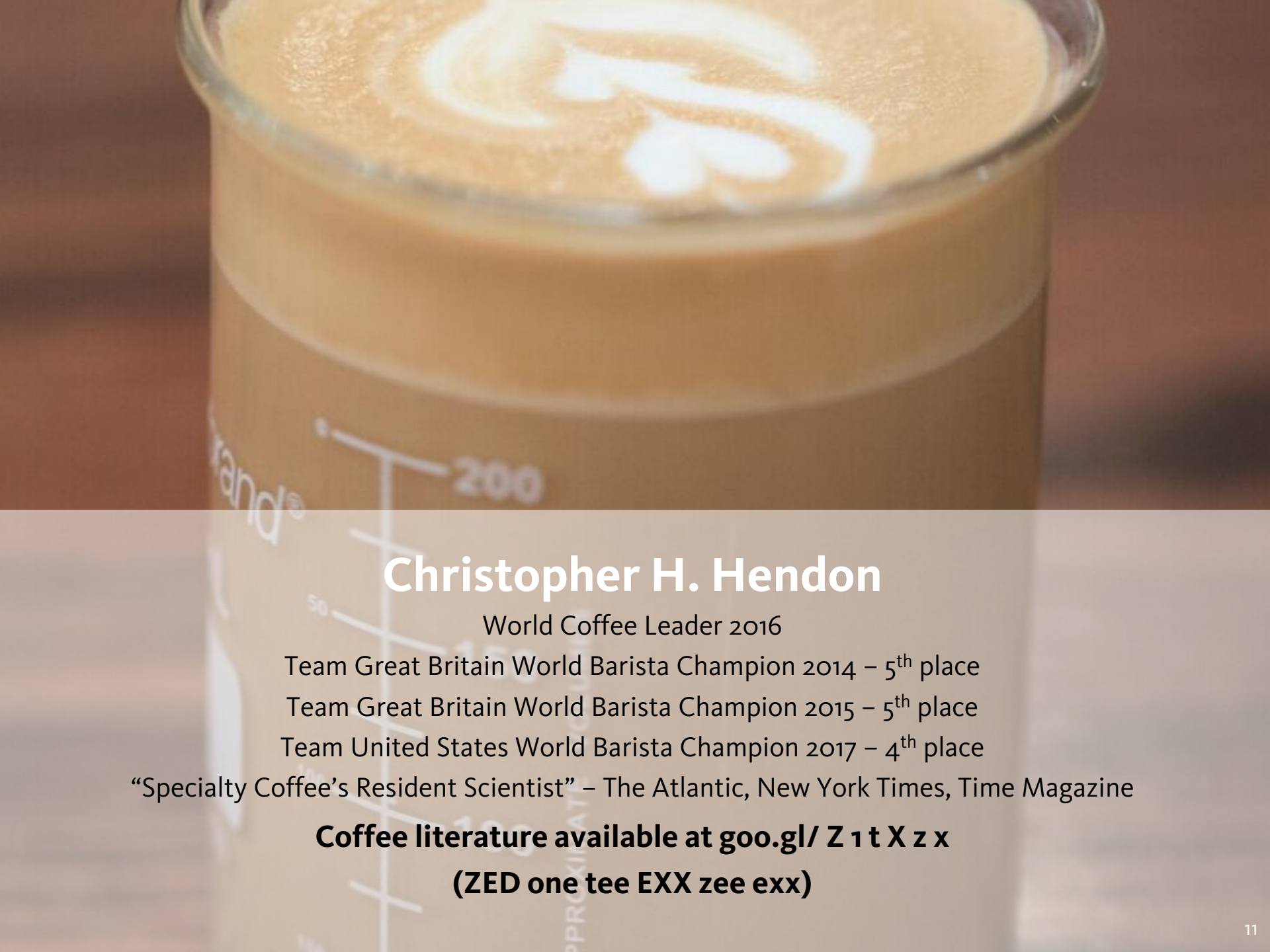
Metal-organic frameworks

Linked together by organic linkers



Single-site heterogeneous catalysis of olefins to their oligomers



A close-up photograph of a glass filled with coffee. The coffee has a thick, light brown foam on top, and a white latte art design is visible on the surface. The glass is partially filled with the coffee liquid. The background is blurred, showing a wooden surface.

Christopher H. Hendon

World Coffee Leader 2016

Team Great Britain World Barista Champion 2014 – 5th place

Team Great Britain World Barista Champion 2015 – 5th place

Team United States World Barista Champion 2017 – 4th place

“Specialty Coffee’s Resident Scientist” – The Atlantic, New York Times, Time Magazine

Coffee literature available at [goo.gl/ Z 1 t X z x](https://goo.gl/Z1tXzx)

(ZED one tee EXX zee exx)

The beginning of my coffee journey – Colonna and Smalls, Bath UK

ESPRESSO

PASSEIRO
- BRAZIL -

RUBI
VARIETY
NATURAL

TASTING NOTES
FOR ESPRESSO SHOT

FRUIT CAKE,
BRANDY,
TOASTED SEEDS.

TASTING NOTES
FOR FLAT WHITE

DARK TOFFEE,
COCOA,
CUSTARD,
BRAZIL NUT.

BUF COOP, NYARUSIZA
- RWANDA -

RED BOURBON
WASHED

TASTING NOTES
FOR ESPRESSO SHOT

TREACLE, BERRIES,
SPICE
CANDIED ORANGE
PORT.

TASTING NOTES
FOR FLAT WHITE

TOFFEE,
BISCUIT,
SALT CARAMEL,
DARK CHOCOLATE.

EL VERGIL
- COLOMBIA -

CATURRA
VARIETY
WASHED

TASTING NOTES
FOR ESPRESSO SHOT

BOILED SWEETS,
TREACLE,
BLACKBERRY,
CHOCOLATE,
SWEET SPICE.

TASTING NOTES
FOR FLAT WHITE.

CASSIS,
CHOCOLATE,
HAZELNUT,
CREME CARAMEL.

FILTER

RECOMMENDED BLACK

FINCA KASSANDRA
- MEXICO -

PANAMA
VARIETY
WASHED

RED CURRANT,
BLUEBERRY, CHOCOLATE,
APPLE.

REMEDI NYAMAGABE
- RWANDA -

WASHED

20P
EXTRA

LIME, FLORAL,
BLACKBERRY, COCOA,
HERBAL.

SANTA GEMA - MARACATURRA
- NICARAGUA -

WASHED

RASPBERRY, SILKY,
MINERAL,
CHOCOLATE, WALNUT.

The aim

reproducibly flavorsome coffee



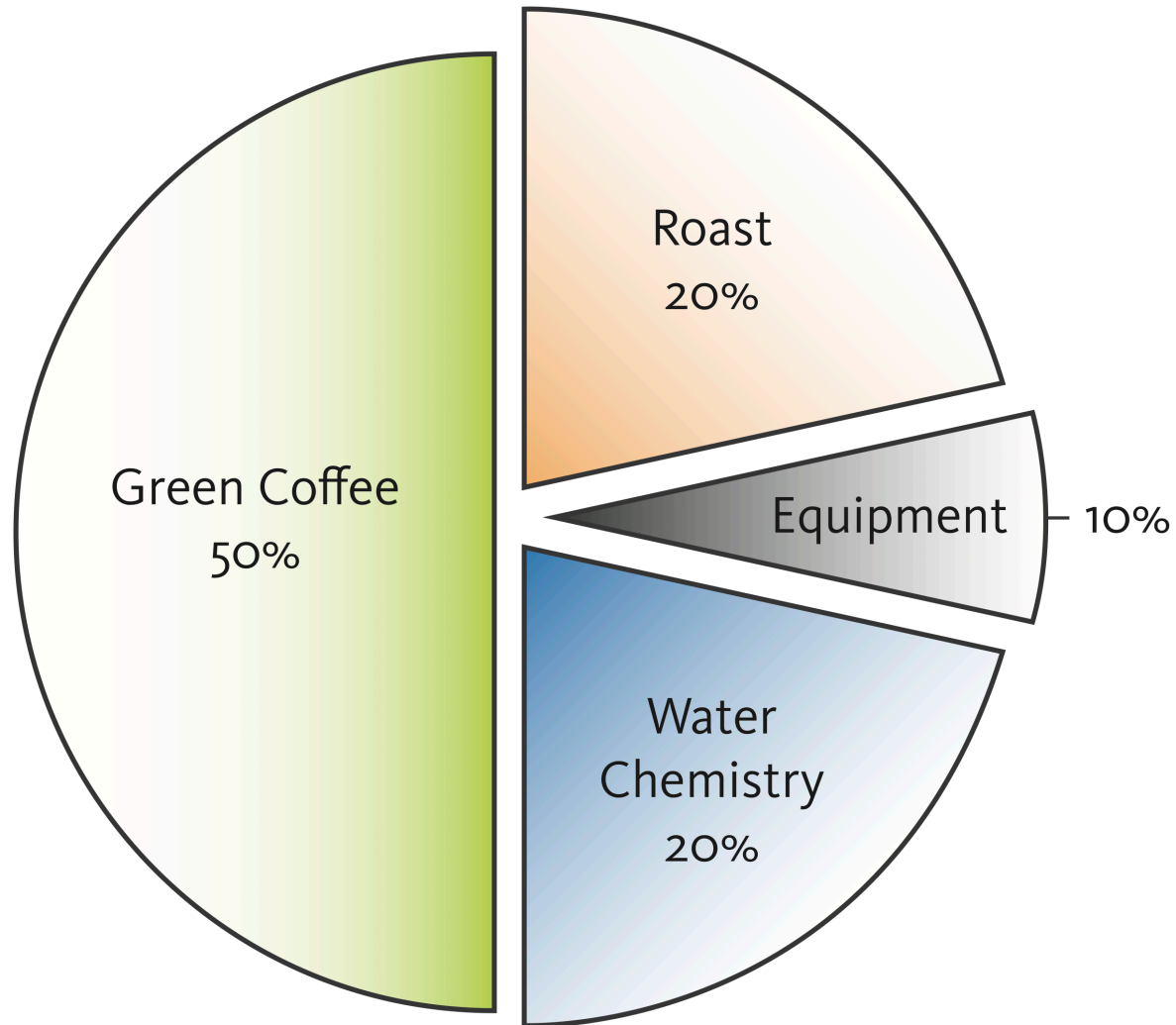
The disappointment

an occasional flavor malfunction





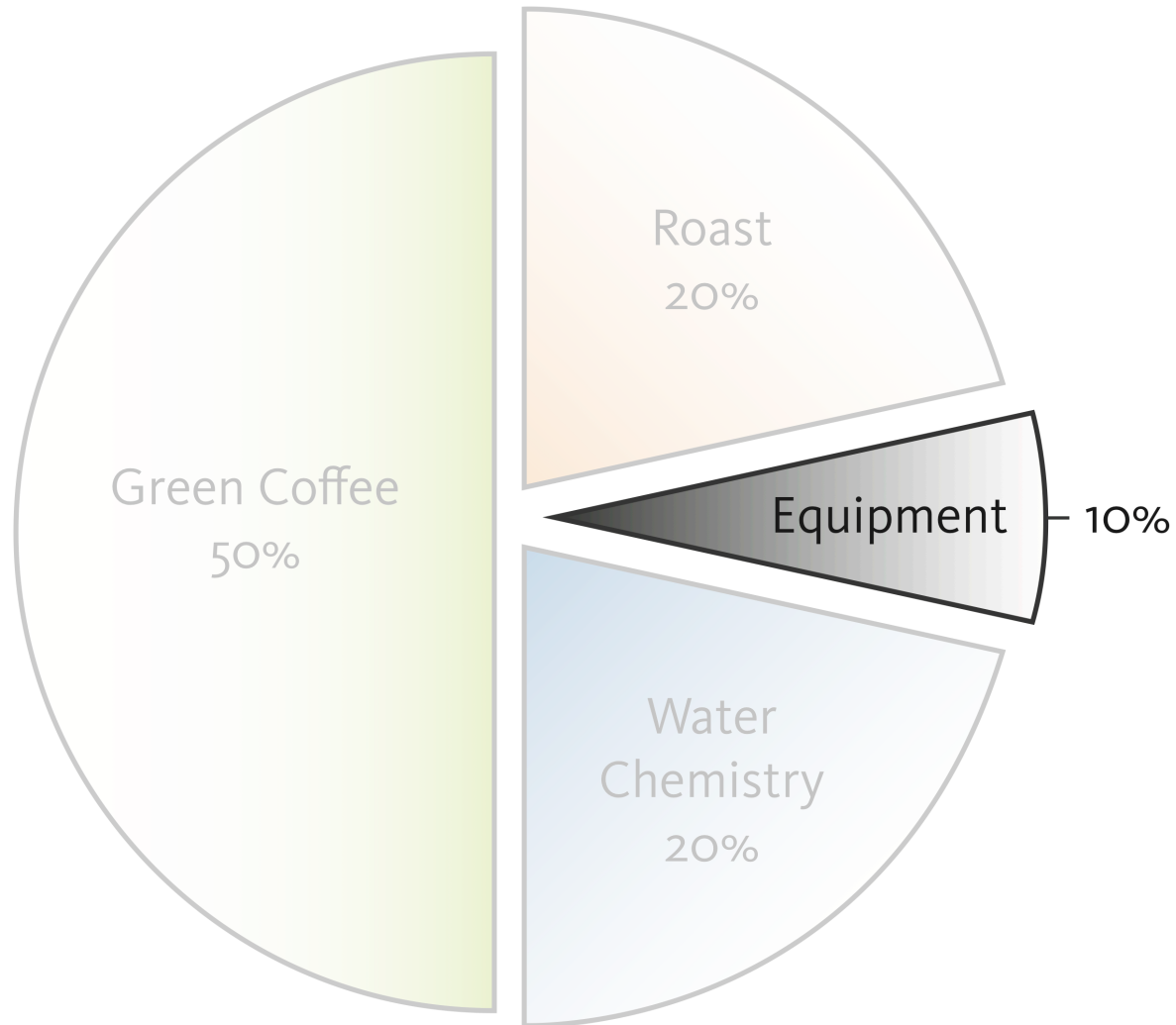
Contributors to a quality cup of coffee*



* Of course something could go wrong at every stage of brewing.
This figure is rather used to emphasize that quality coffee is less dependent on the brew method.



Contributors to a quality cup of coffee*



* Of course something could go wrong at every stage of brewing.
This figure is rather used to emphasize that quality coffee is less dependent on the brew method.



Coffee is graded on the cupping table

No equipment, just water, coffee coarsely ground, and a spoon + 4 min brew time





Agriculture and Economics



Coffee market analysis

1.3% of USA GDP (\$225.2B in 2015)

“Drip” (i.e. filter) coffee dominates the USA

Drip is 1.2 – 1.5 % w/w

Espresso-based beverages prolific in Europe

Espresso is 8 – 10 % w/w

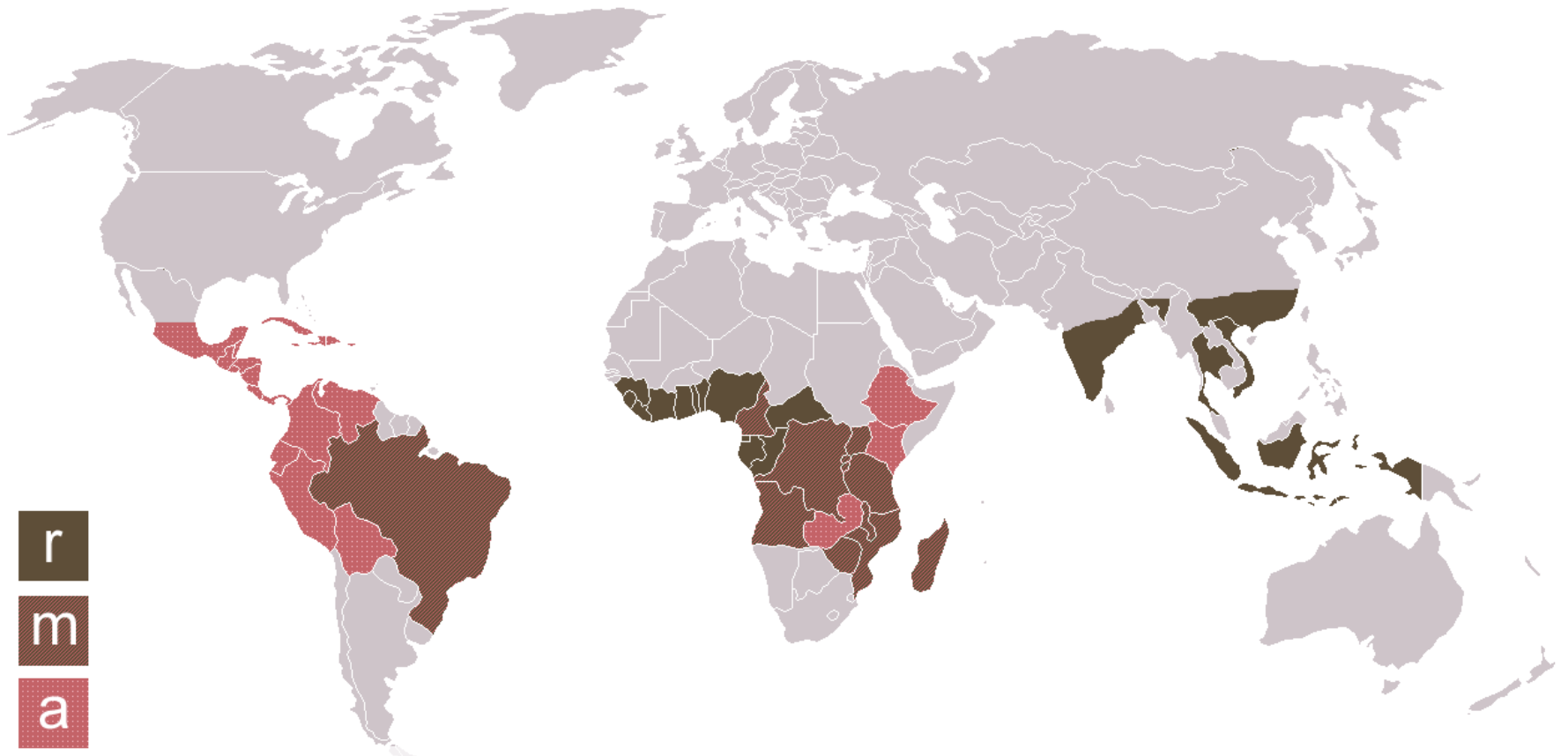
Coffee is kind of a big deal to other countries, too:

Burundi — 25% GDP (~\$8B) is coffee, 90% population employed



The Bean Belt

The balance between low CO₂ concentrations and high temperature



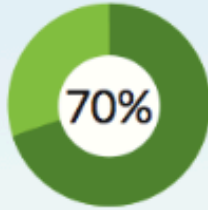
Microclimates are extremely important, and very poorly studied.



ARABICA



ALTITUDE



WORLD PRODUCTION



SUSCEPTIBLE



NEED ATTENTION

In higher demand because it tastes “better”

ROBUSTA



ALTITUDE



WORLD PRODUCTION



HARDY



HIGH IN CAFFEINE

1250m

1000m

750m

500m

250m

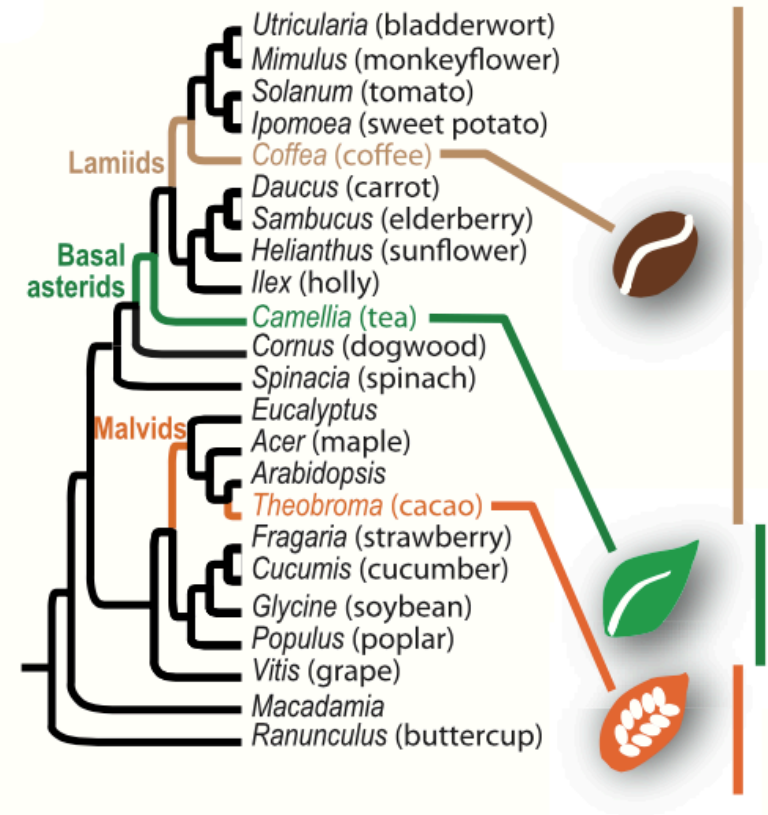
SEA LEVEL

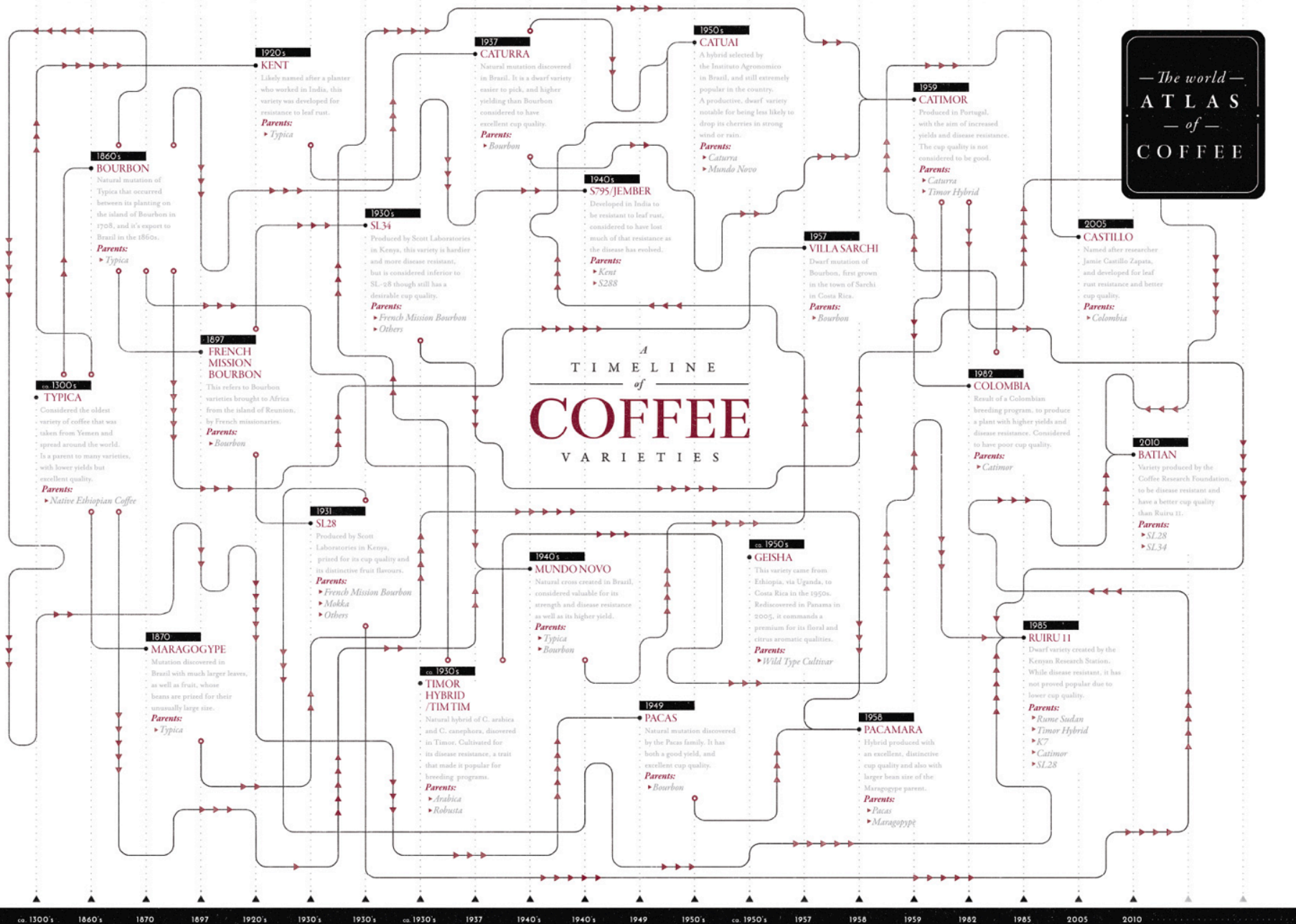
We have the genome for both Robusta and Arabica

PLANT GENOMICS

The coffee genome provides insight into the convergent evolution of caffeine biosynthesis

France Denoeud,^{1,2,3} Lorenzo Carretero-Paulet,⁴ Alexis Dereeper,⁵ Gaëtan Droc,⁶ Romain Guyot,⁷ Marco Pietrella,⁸ Chunfang Zheng,⁹ Adriana Alberti,¹ François Anthony,⁵ Giuseppe Aprea,⁸ Jean-Marc Aury,¹ Pascal Bento,¹ Maria Bernard,¹ Stéphanie Bocs,⁶ Claudine Campa,⁷ Alberto Cenci,^{5,10} Marie-Christine Combes,⁵ Dominique Crouzillat,¹¹ Corinne Da Silva,¹ Loretta Daddiego,¹² Fabien De Bellis,⁶ Stéphane Dussert,⁷ Olivier Garsmeur,⁶ Thomas Gayraud,⁷ Valentin Guignon,¹⁰ Katharina Jahn,^{9,13,14} Véronique Jamilloux,¹⁵ Thierry Joët,⁷ Karine Labadie,¹ Tianying Lan,^{4,16} Julie Leclercq,⁶ Maud Lepelley,¹¹ Thierry Leroy,⁶ Lei-Ting Li,¹⁷ Pablo Librado,¹⁸ Loredana Lopez,¹² Adriana Muñoz,^{19,20} Benjamin Noel,¹ Alberto Pallavicini,²¹ Gaetano Perrotta,¹² Valérie Poncet,⁷ David Pot,⁶ Priyono,²² Michel Rigoreau,¹¹ Mathieu Rouard,¹⁰ Julio Rozas,¹⁸ Christine Tranchant-Dubreuil,⁷ Robert VanBuren,¹⁷ Qiong Zhang,¹⁷ Alan C. Andrade,²³ Xavier Argout,⁶ Benoît Bertrand,²⁴ Alexandre de Kochko,⁷ Giorgio Graziosi,^{21,25} Robert J Henry,²⁶ Jayarama,²⁷ Ray Ming,¹⁷ Chifumi Nagai,²⁸ Steve Rounsley,²⁹ David Sankoff,⁹ Giovanni Giuliano,⁸ Victor A. Albert,^{4*} Patrick Wincker,^{1,2,3*} Philippe Lashermes^{5*}





Coffee begins life as a fruit

Inevitably the fruit is removed to yield a green seed (~11% moisture content)



Fruit or mucilage

Parchment

Seed



Processing methods

The stage in which coffee is dried

Natural process



Fruit or mucilage

Pulped



Washed process



Parchment

Seed

The chemistry of each processing method is widely unknown

All coffee is then fermented for ~24 hours



Naturals historically came from places with water scarcity or environment in mind

Yemen, parts of Ethiopia, and more recently Brazil



A drying facility in Ethiopia



Defective naturals are UV active
Why?



The '*best*' coffees in the world

Kopi Luwak (Civet) — fallacy





The '**best**' coffees in the world

fact

No particular country dependence

Although Brazilian, Sumatran, Vietnamese and Hawaii are typically the lowest scoring

Panama Geishas are typically the award winners

Natural and Washed





Specialty Coffee Association of America Cupping Form

Name: _____

Date: _____ Table: _____ Session: _____

Classification:

6.00 - Good	7.00 - Very Good	8.00 - Excellent	9.00 - Outstanding
6.25	7.25	8.25	9.25
6.50	7.50	8.50	9.50
6.75	7.75	8.75	9.75

Sample #	Roast level	Fragrance/Aroma	Flavor	Acidity	Body	Uniformity	Clean Cup	Overall	Total Score
		Total: 6 7 8 9 10 Dry Quality: Crust:	Total: 6 7 8 9 10 Aftertaste	Total: 6 7 8 9 10 Intensity High Low	Total: 6 7 8 9 10 Intensity High Low	Total: 6 7 8 9 10 Balance	Total: 6 7 8 9 10 Sweetness	Total: 6 7 8 9 10 Defects (subtract)	
Notes: _____									Final Score

Sample #	Roast level	Fragrance/Aroma
		Total: 6 7 8 9 10 Dry Quality: Crust:
Notes: _____		



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6.75	7.75	8.75	9.75

Sample #	Roast level	Fragrance/Aroma	Flavor	Acidity	Body	Uniformity	Clean Cup	Overall	Total Score
		Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total:
		Dry Quality: Crust:	Total: 6 7 8 9 10	Intensity High Low	Intensity High Low	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Defects (subtract) Taint=2 Fault=4	# of cups Intensity X =
Notes:									Final Score

Total: Flavor 6 7 8 9 10	Total: Acidity 6 7 8 9 10
Total: Aftertaste 6 7 8 9 10	Intensity High Low



Specialty Coffee Association of America Cupping Form

Name: _____

Date: _____ Table: _____ Session: _____

Classification:

6.00 - Good	7.00 - Very Good	8.00 - Excellent	9.00 - Outstanding
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Sample #	Roast level	Fragrance/Aroma	Flavor	Acidity	Body	Uniformity	Clean Cup	Overall	Total Score
		Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total: 6 7 8 9 10	Total:
		Dry Quality: Crust:	Aftertaste Total: 6 7 8 9 10	Intensity High Low	Intensity High Low	Balance Total: 6 7 8 9 10	Sweetness ☐ ☐ ☐ ☐ ☐	Defects (subtract) Taint=2 Fault=4 # of cups Intensity ☐ X ☐ =	
Notes: _____									Final Score

Total: Body 6 7 8 9 10 Intensity High Low	Total: Uniformity ☐ ☐ ☐ ☐ ☐ Total: Balance 6 7 8 9 10
--	--



Specialty Coffee Association of America Cupping Form

Name: _____

Date: _____ Table: _____ Session: _____

Classification:

6.00 - Good	7.00 - Very Good	8.00 - Excellent	9.00 - Outstanding
6.25	7.25	8.25	9.25
6.50	7.50	8.50	9.50
6.75	7.75	8.75	9.75

Sample #	Roast level	Fragrance/Aroma	Flavor	Acidity	Body	Uniformity	Balance	Clean Cup	Overall	Total Score	
		Dry Quality: Crust:	Aftertaste	Intensity High Low	Intensity High Low		Balance		Defects Taint=2 Fault=4	# of cups Intensity X =	
Notes:										Final Score	

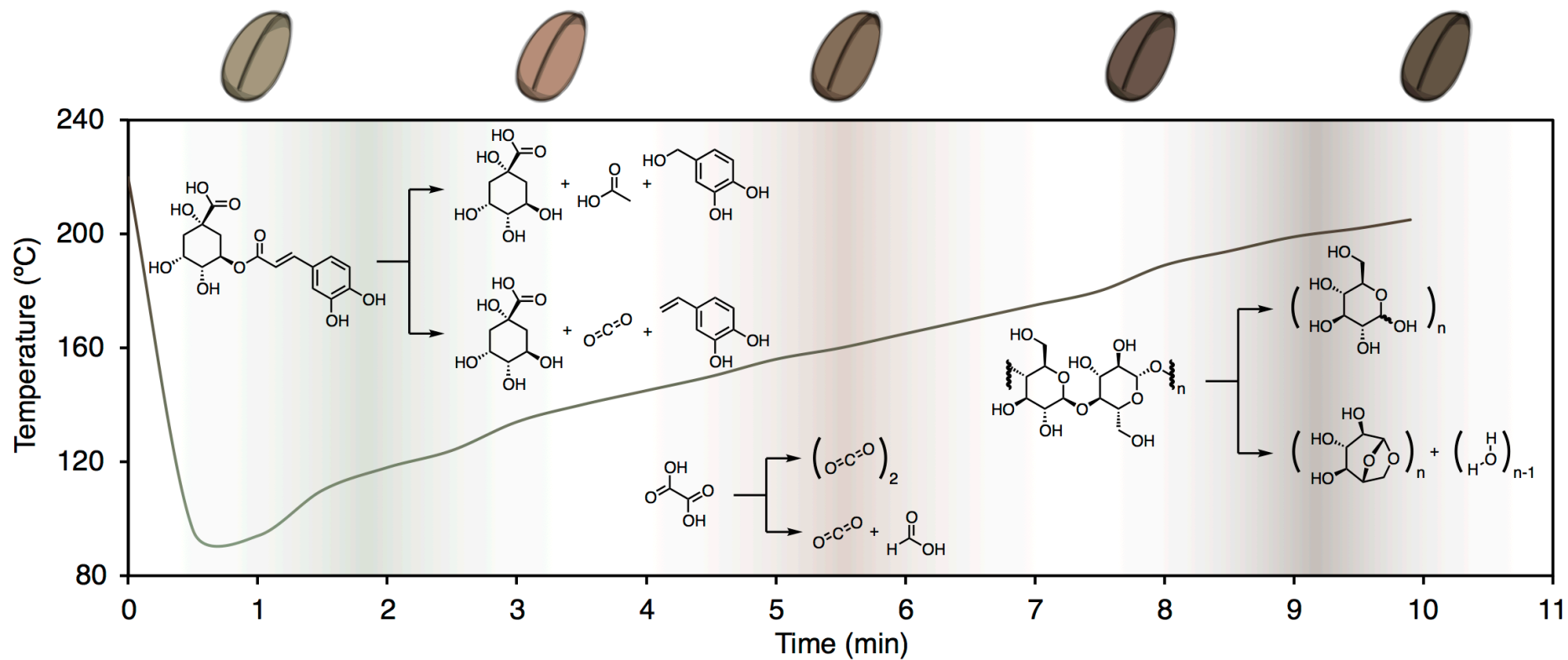
Clean Cup:	Overall	Total Score
Sweetness	Defects (subtract) Taint=2 Fault=4 X =	

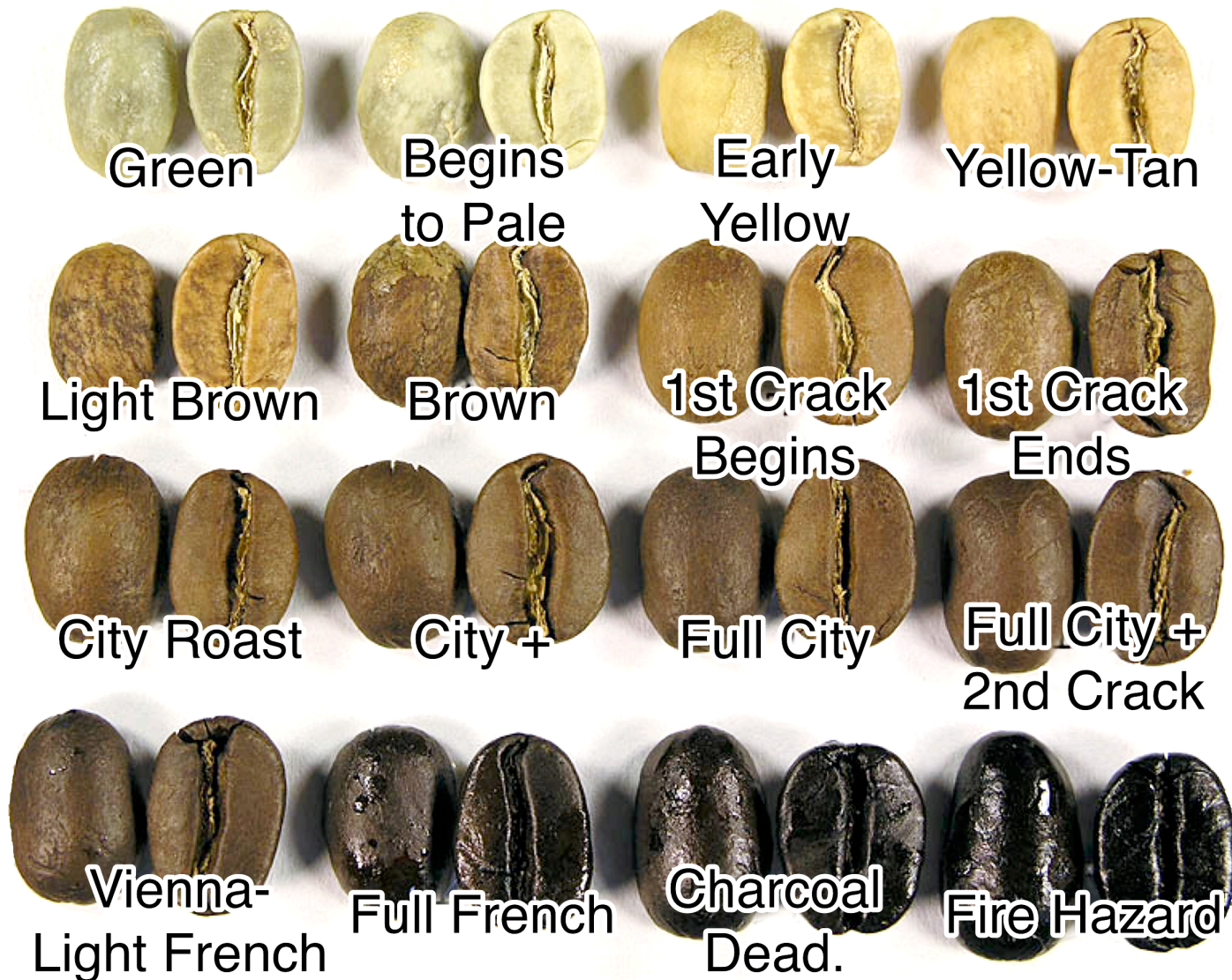


Roasting

The roast profile

Kinetics: Gradient and time determine flavor development





Dark* roasted coffee is a good ORR catalyst

*dark = 800 °C, ZnCl₂, Ar

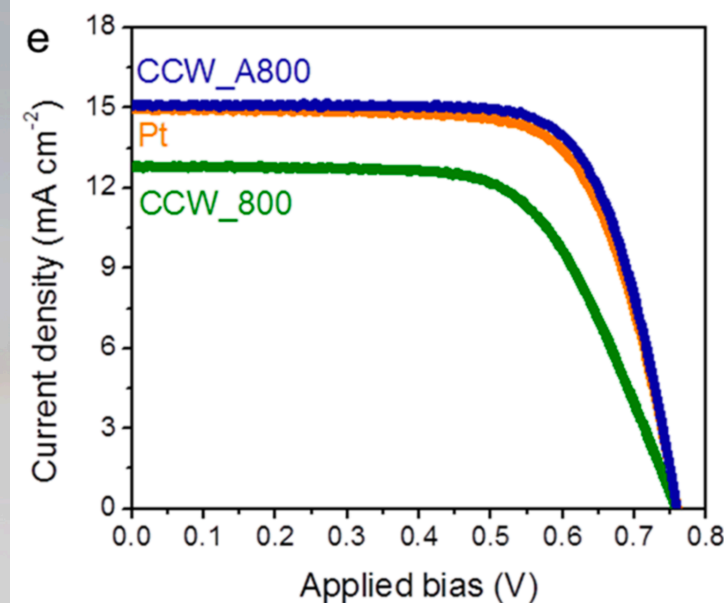


Figure 1. Scheme of coffee waste-derived hierarchical nitrogen-doped porous carbon synthesis.



Dark roast coffee contains more caffeine?

Fallacy

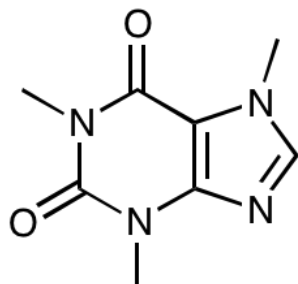


Table II. Caffeine Content of Espresso and Brewed Specialty Coffees

Coffee and Origin	Amount	Caffeine Dose (mg)
Espresso coffees		
Big Bean Espresso, 1-shot	1 shot	75.8
Big Bean Espresso, 2 short shots	2 short shots	140.4
Big Bean Espresso, 2 tall shots	2 tall shots	165.3
Starbucks Espresso, regular, small	1 shot	58.1
Hampden Café Espresso	2 shots	133.5
Einstein Bros® Espresso, double	2 shots	185.0

Brewed specialty coffees

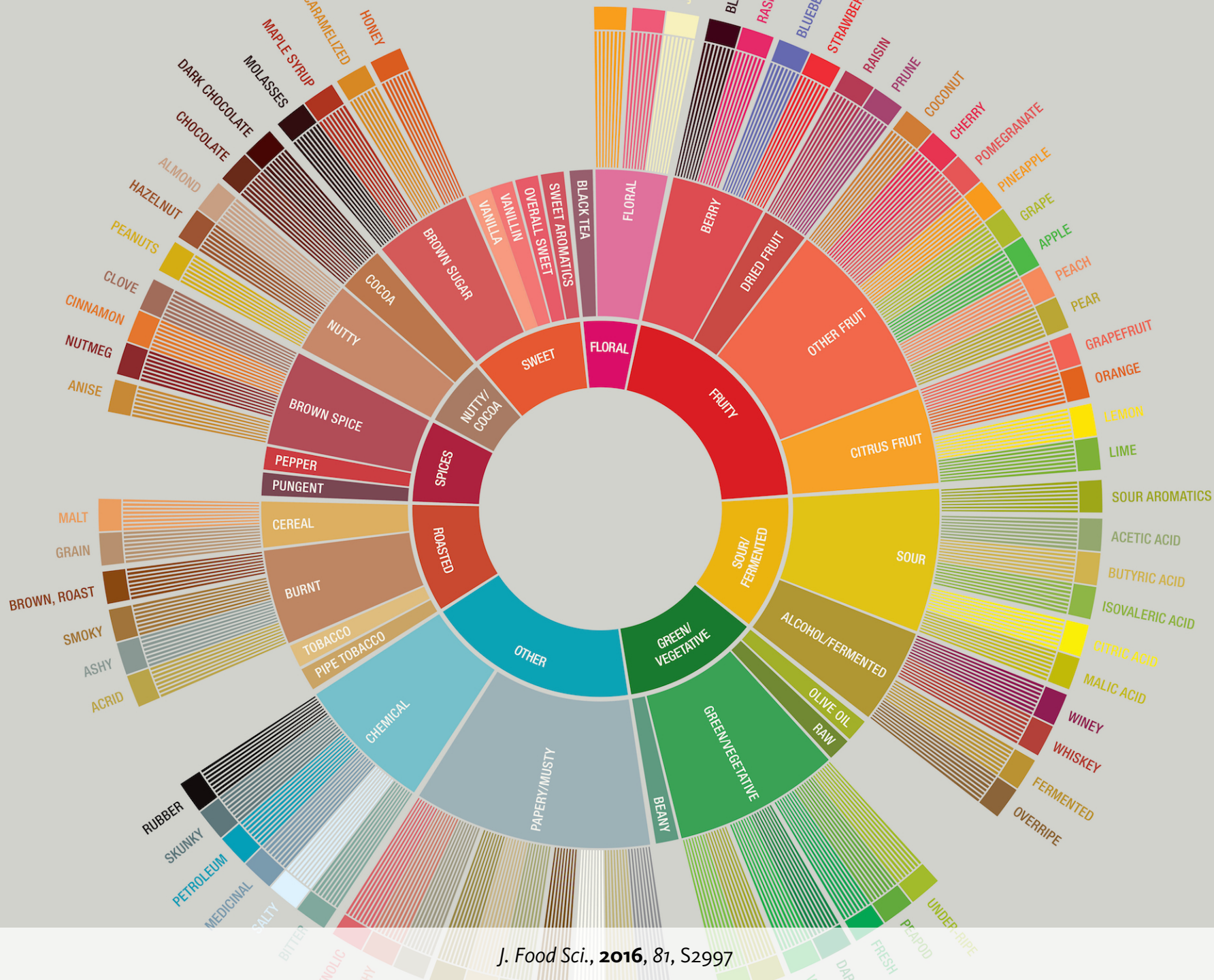
Big Bean, regular	16 oz	164.7
Big Bean Boat Builders Blend, regular	16 oz	147.6
Big Bean Organic Peru Andes Gold, regular, country origin, Peru	16 oz	186.0
Big Bean French Roast, regular	16 oz	179.8
Big Bean Ethiopian Harrar, regular, country origin, Ethiopia	16 oz	157.1
Big Bean Italian Roast, regular, country origin, Brazil	16 oz	171.8
Big Bean Costa Rican French Roast, regular, country origin, Costa Rica	16 oz	245.1
Big Bean Kenya AA, regular, country origin, Kenya	16 oz	204.9
Big Bean Sumatra Mandheling, regular, country origin, Indonesia	16 oz	168.5
Hampden Café Guatemala Antigua	16 oz	172.7
Starbucks regular	16 oz	259.3
Royal Farms regular	16 oz	225.7
Dunkin' Donuts regular	16 oz	143.4
Einstein Bros regular	16 oz	206.3



Some chemistry in roasted coffee

Table I. Coffee Volatiles Identified in the Present Investigation^a

Compound	References	Compound	References
Hydrocarbons		Lactones	
Isoprene	Rhoades, 1958, 1960	γ -Butyrolactone	Viani <i>et al.</i> , 1965
Alcohols		γ -Valerolactone	
Methanol	Reichstein and Staudinger, 1962b	α -Methyl- γ -butyrolactone	
Ethanol	Rhoades, 1958, 1960	2,3-Dimethylbut-2-en-1,4-olide	
2-Propanol		3,4-Dimethylbut-2-en-1,4-olide	
3-Methylbut-2-en-1-ol	Stoll <i>et al.</i> , 1967	2,3,4-Trimethylbut-2-en-1,4-olide	
Linalool	Stoll <i>et al.</i> , 1967		
<i>cis</i> -Linalool oxide	Stoll <i>et al.</i> , 1967		
<i>trans</i> -Linalool oxide			
Aldehydes		Esters	
Ethanal	Reichstein and Staudinger, 1926b	Methyl formate	Rhoades, 1958, 1960
Propanal	Zlatkis and Sivetz, 1960	Methyl acetate	Sullivan <i>et al.</i> , 1959
2-Methylpropanal	Rhoades, 1958, 1960	Methyl propionate	Merritt <i>et al.</i> , 1966
<i>n</i> -Butanal	Rhoades, 1958, 1960	Methyl salicylate	Stoll <i>et al.</i> , 1967
3-Methylbutanal	Rhoades, 1958, 1960	Methyl phenylacetate	
2-Methylbutanal	Reichstein and Staudinger, 1926b	Ethyl formate	Zlatkis and Sivetz, 1960
<i>n</i> -Pentanal	Zlatkis and Sivetz, 1960	Ethyl acetate	Gianturco <i>et al.</i> , 1966
2-Methylbut-2-en-1-al	Sullivan <i>et al.</i> , 1959	Isopropyl formate	
<i>m</i> -Tolualdehyde (tentative)		Isoamyl acetate	
Ketones		β -Phenylethyl formate	Stoll <i>et al.</i> , 1967
Propanone	Bernheimer, 1880	Phenols and Phenol Ethers	
Butanone	Rhoades, 1958, 1960	Phenol	Reichstein and Staudinger, 1926b
3-Hexanone	Stoll <i>et al.</i> , 1967	<i>o</i> -Cresol	Stoll <i>et al.</i> , 1967
<i>trans</i> -2-Penten-4-one		2,6-Dimethylphenol	Stoll <i>et al.</i> , 1967
Cyclopentanone	Gianturco <i>et al.</i> , 1966	Guaiacol	Reichstein and Staudinger, 1926b
Hexane-2,5-dione		4-Ethylguaiacol	Gianturco <i>et al.</i> , 1966
Heptane-2,5-dione		4-Vinylguaiacol	Reichstein and Staudinger, 1926b
		<i>o</i> -Hydroxyacetophenone	Stoll <i>et al.</i> , 1967
		Sulfur-containing	

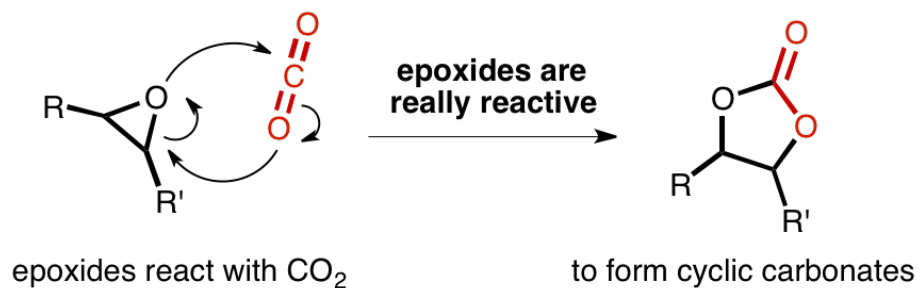




J. Agric. Food Chem., **2003**, 51, 4782

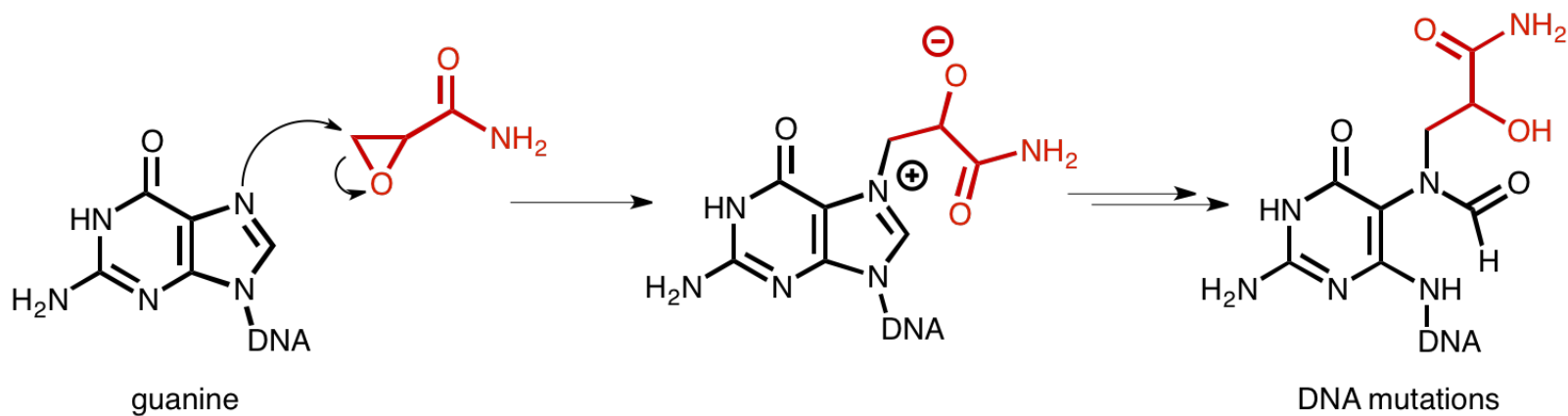
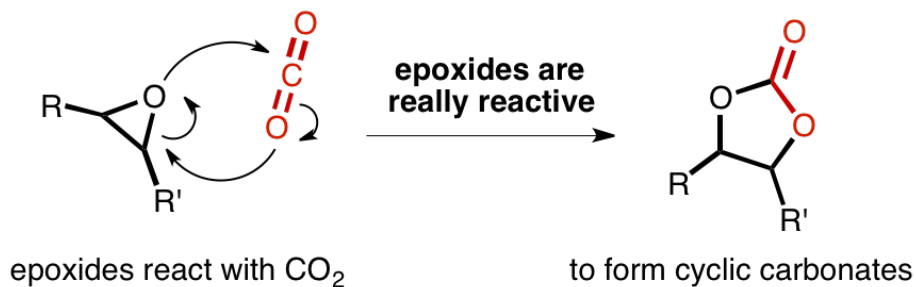


J. Agric. Food Chem., **2003**, 51, 4782





J. Agric. Food Chem., **2003**, 51, 4782





Does acrylamide cause cancer?

Does coffee cause cancer?

If something causes cancer it needs to show an increase in cancer rates of 1 in 100,000 people

Of the 100,000 people **50,000 people will likely develop cancer anyway** unrelated to acrylamide of coffee

Hence, a sample size of **85 billion people** required to make conclusive statement on current population



Death is in the dose and “slope factors”

0.0005 slope factor for acrylamide

Increase in likelihood of cancer with consumption of
1 μ g/kg/day

The average person weighs 70 kg — 70 kg / slope factor
(0.0005).

**An increase in 1 in 140,000 occurrences due to acrylamide
ingestion at 1 μ g/kg/day**

So, how much acrylamide is in a coffee?



~0.5 μg per 6 oz-ish cup

$$0.45 \mu\text{g} * 0.0005 / 70 \text{ kg}$$

1 in 311,111 per cup

3 cups per day still satisfactorily over 1
in 100,000



Grinding



Conical vs. flat burrs

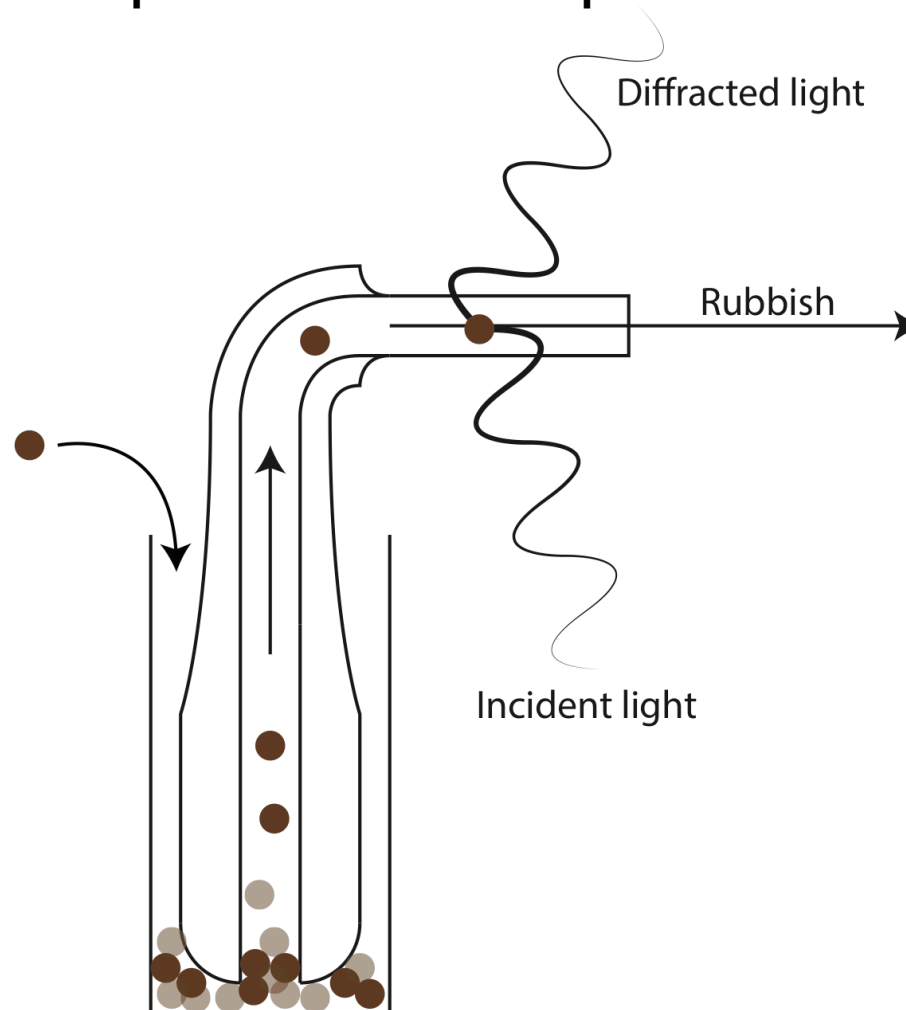
Different burrs produce different particle size distributions





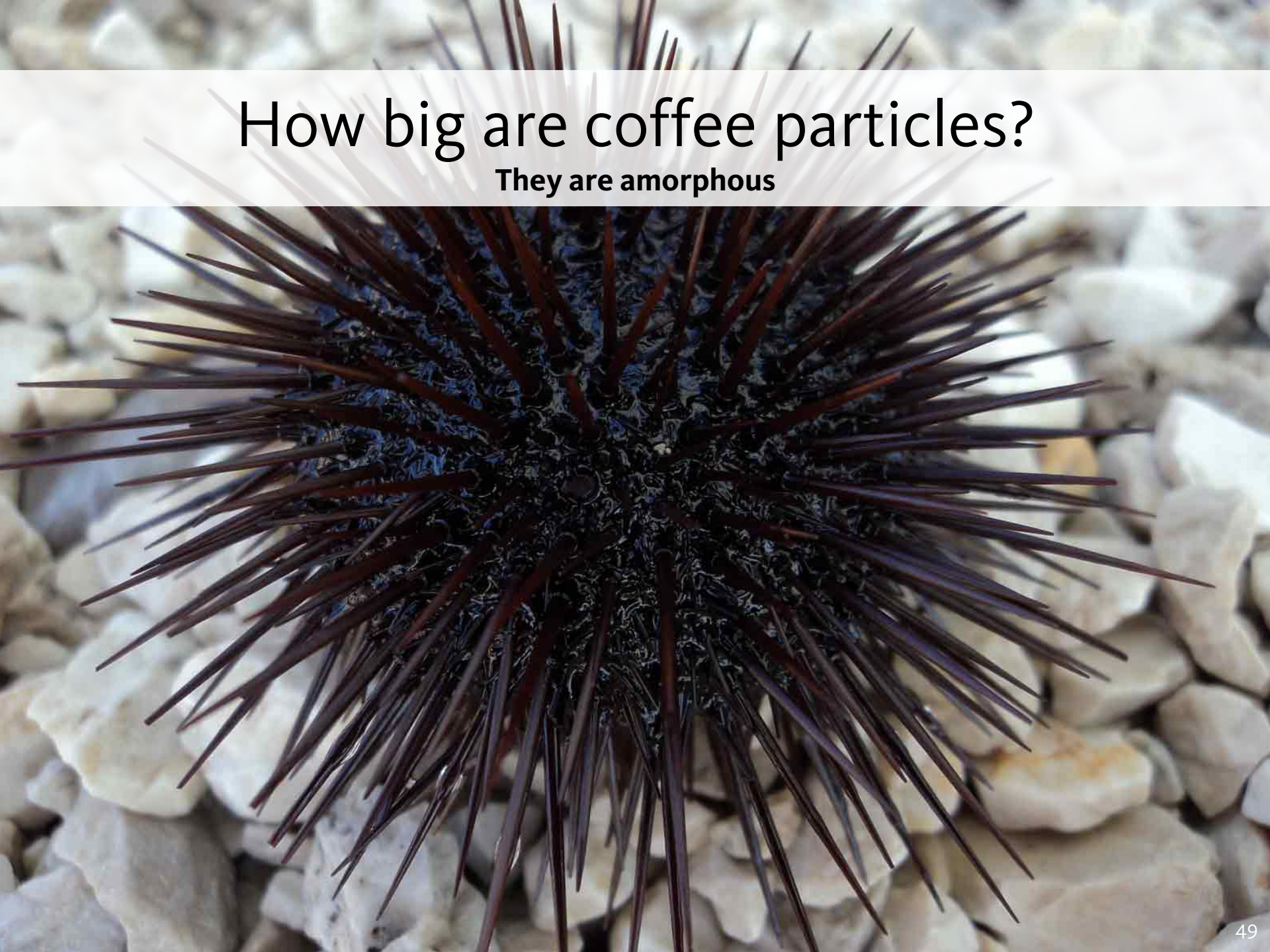
Laser diffraction particle size analysis

A process to determine particle size



How big are coffee particles?

They are amorphous

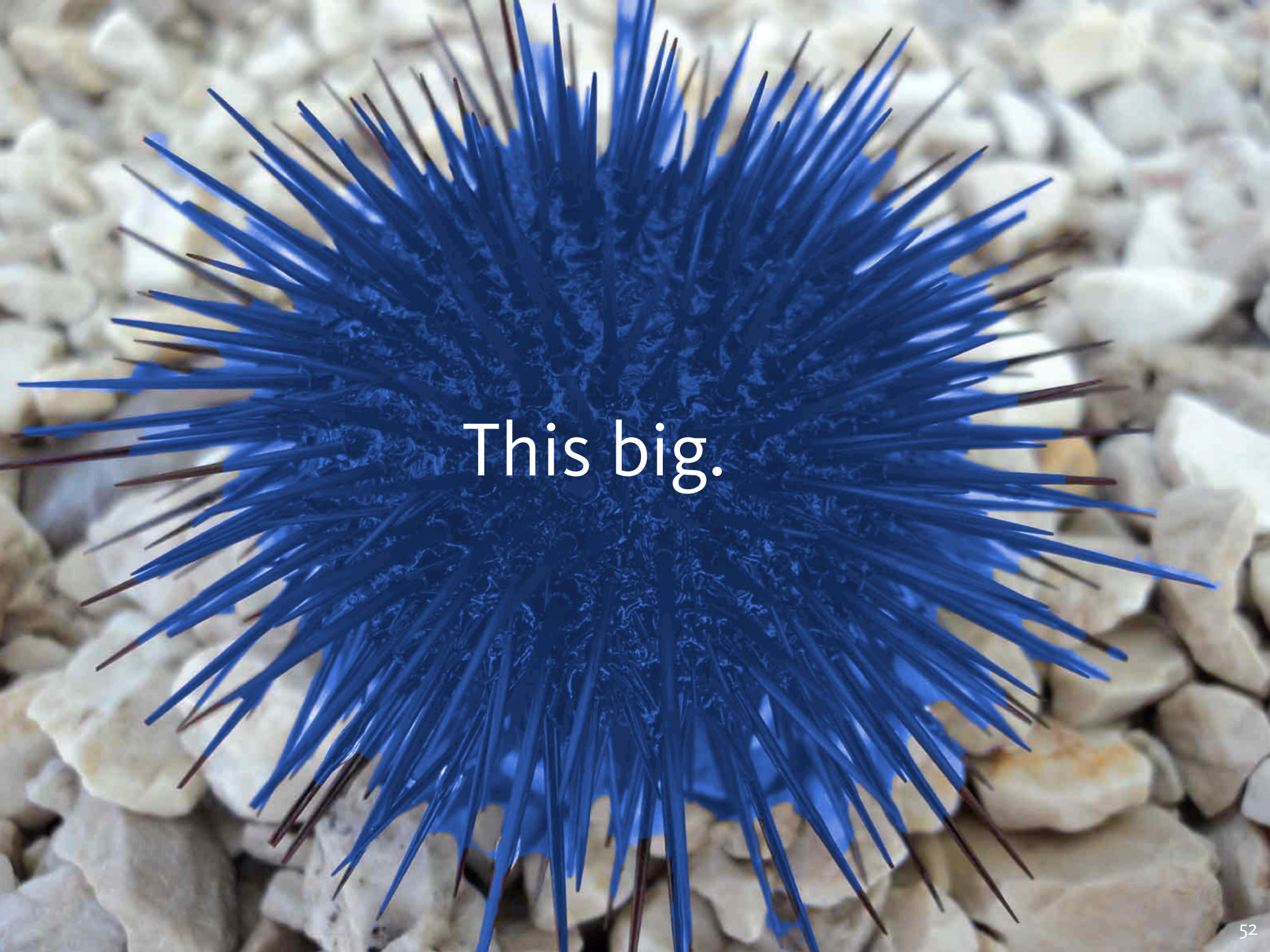


A close-up photograph of a sea urchin resting on a bed of light-colored, irregularly shaped stones. The urchin's body is a dark, almost black, spherical shape covered in numerous long, sharp, dark spines that radiate outwards. A large, semi-transparent red circle is superimposed over the center of the urchin's body. Inside this circle, the text "This big?" is written in a white, sans-serif font.

This big?

A close-up photograph of a sea urchin, showing its numerous sharp, dark spines radiating from a central point. The urchin is resting on a bed of light-colored, irregularly shaped stones. A large, semi-transparent yellow circle is superimposed over the urchin, centered on its body. The text "Or this big?" is written in white, sans-serif font across the middle of the yellow circle.

Or this big?

A close-up photograph of a blue, spiky flower head, possibly a species of thistle or sea urchin, resting on a bed of light-colored, irregularly shaped gravel. The flower head is composed of numerous sharp, blue, needle-like structures radiating from a central point. The text "This big." is overlaid in white, sans-serif font in the center of the image.

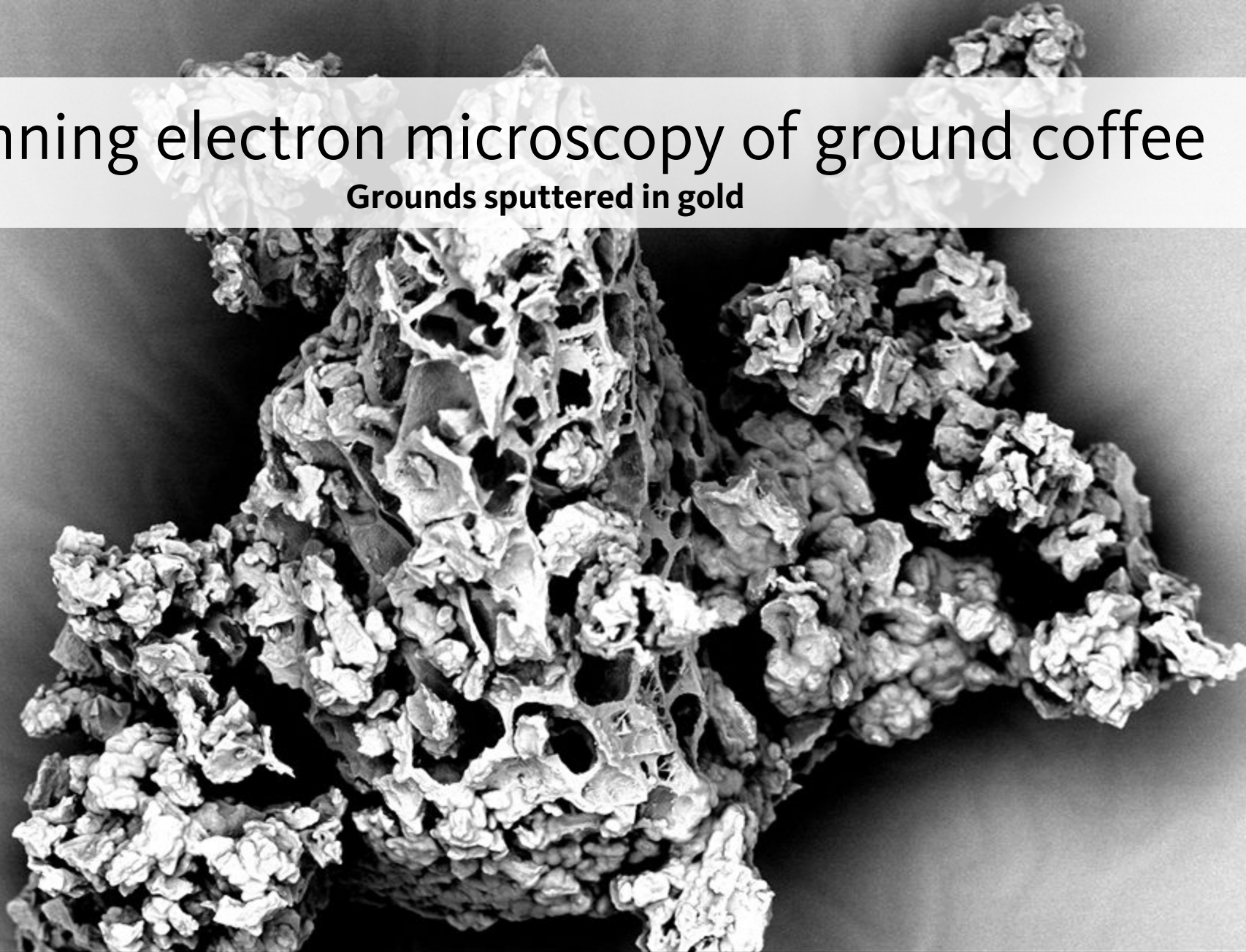
This big.

A close-up photograph of a sea urchin with dark, sharp spines, resting on a bed of light-colored, irregularly shaped rocks. A large, semi-transparent dark circle is superimposed over the urchin, framing the text.

We measure this
conservative surface area to volume

Scanning electron microscopy of ground coffee

Grounds sputtered in gold



BEC 20kV

WD10mm

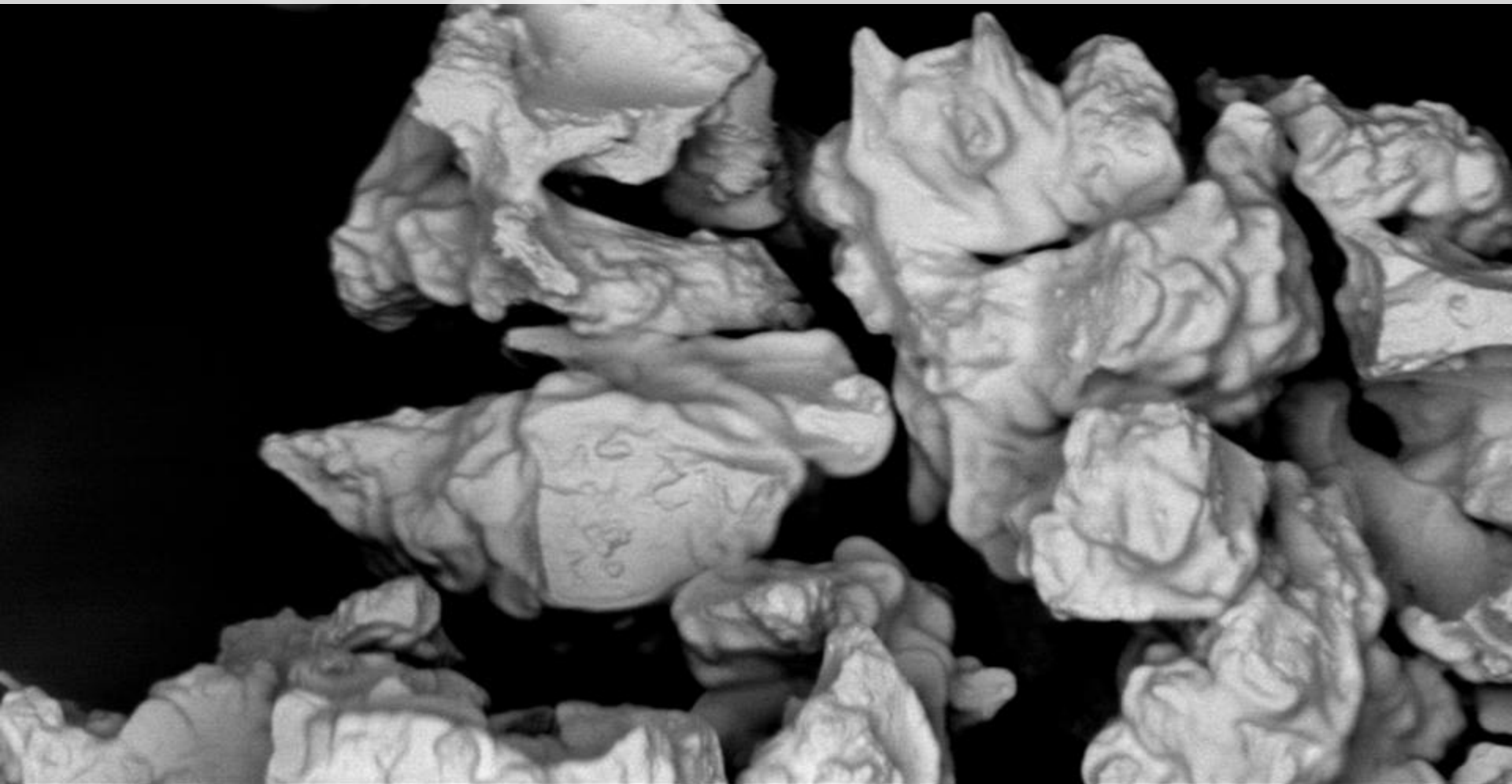
x150

100µm

0000

They don't appear to be very spherical

Grounds sputtered in gold



BEC 10kV

WD10mm

x1,000

10μm

0000





Contents lists available at ScienceDirect

Journal of Food Engineering

journal homepage: www.elsevier.com/locate/jfoodeng

A new methodology to estimate the steady-state permeability of roast and ground coffee in packed beds

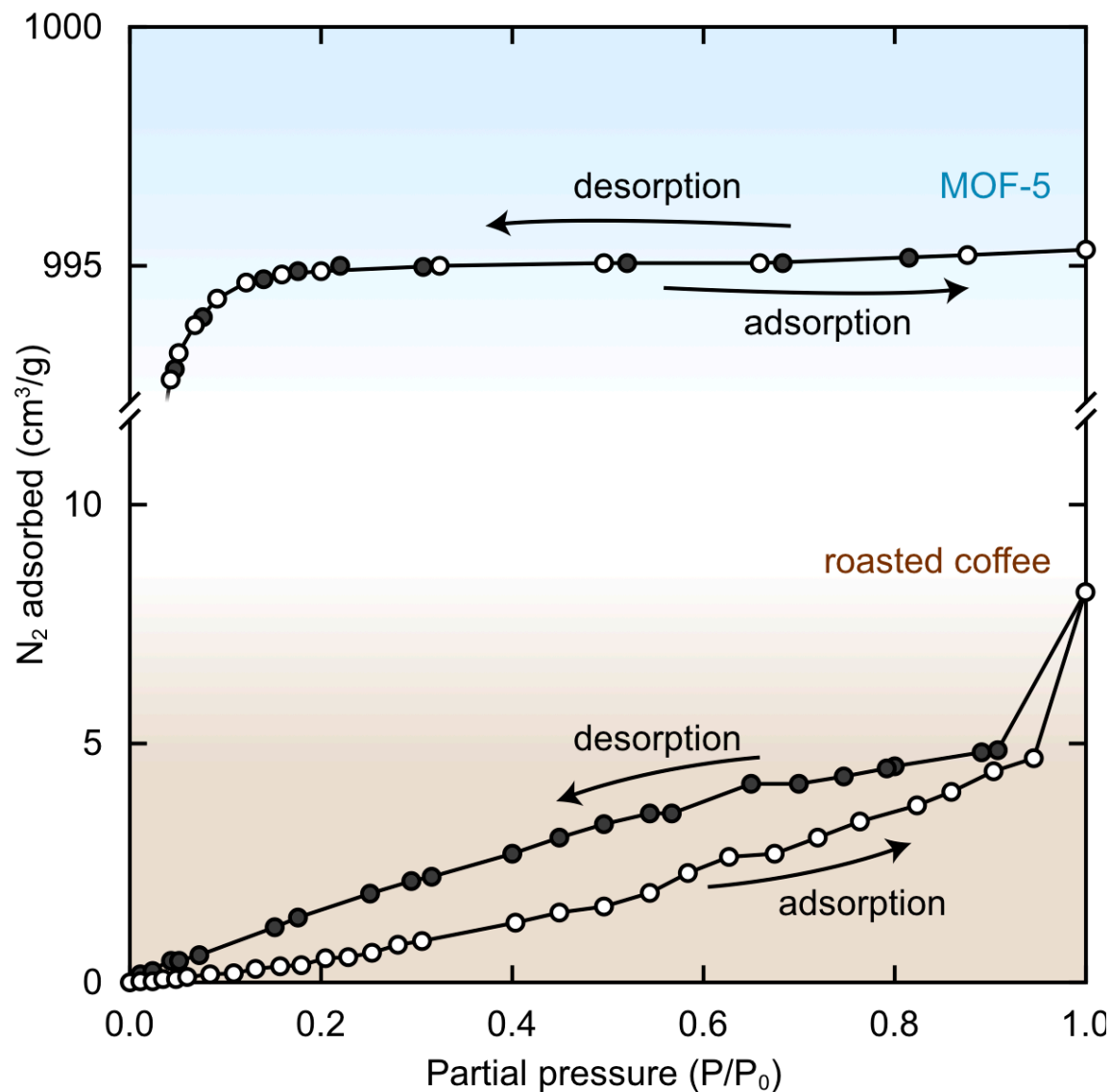


B.R. Corrochano^{a,b,*}, J.R. Melrose^b, A.C. Bentley^b, P.J. Fryer^a, S. Bakalis^a

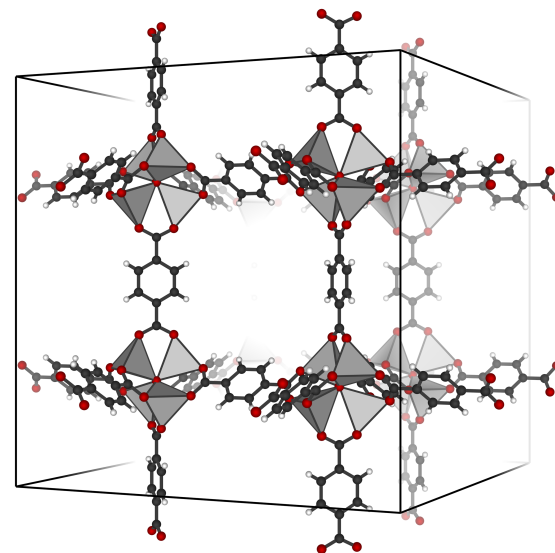
^a Centre for Formulation Engineering, Department of Chemical Engineering, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK

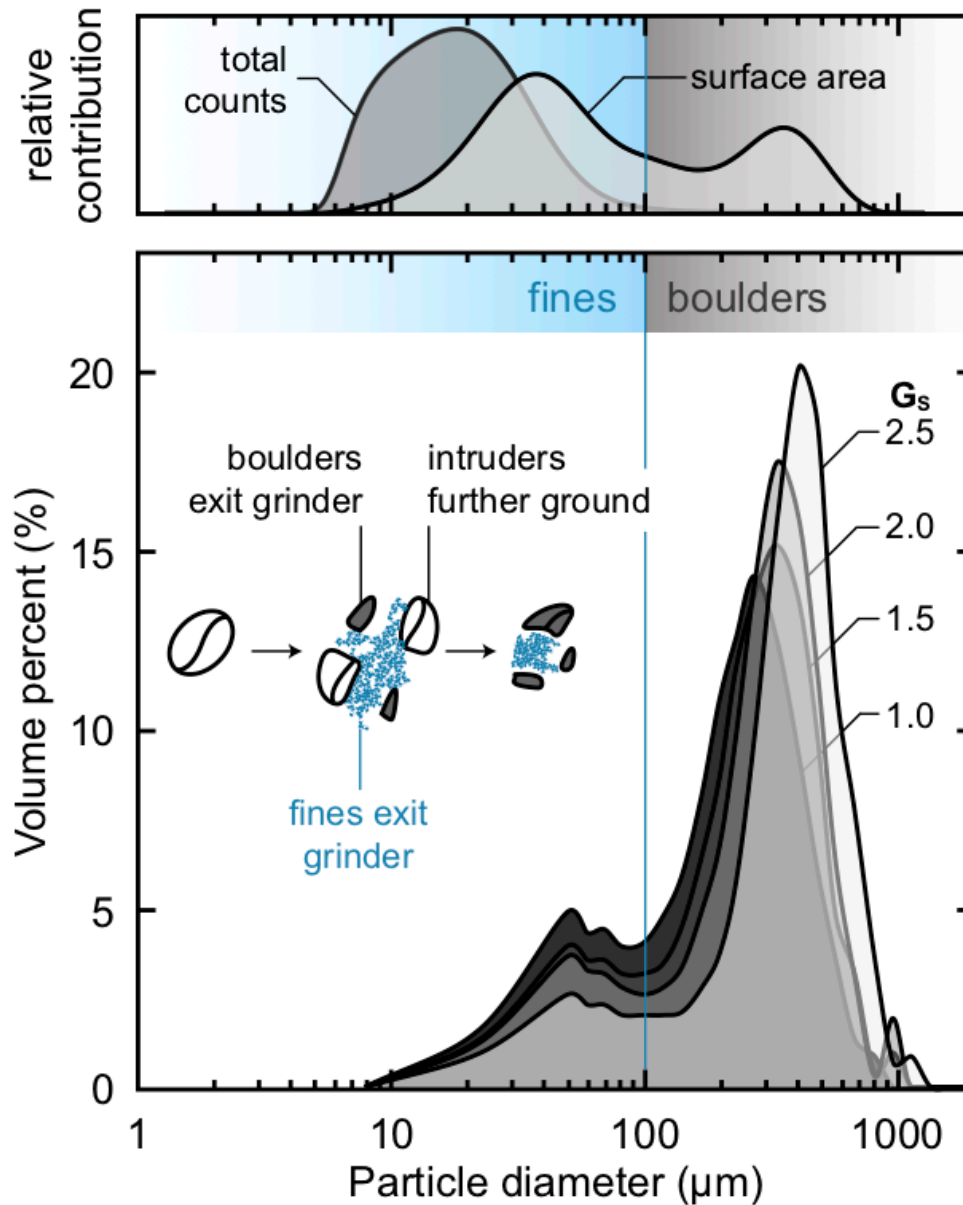
^b Mondelēz International, Coffee Global Centre of Excellence, Ruscott Avenue, Banbury OX16 2QU, UK

- Little particles are closely approximated by a sphere
- Coffee **is** a bit porous (BET measurements are ongoing)
- **Spherical approximation is good enough**



Coffee is
not overly
porous
perhaps
macroporous?

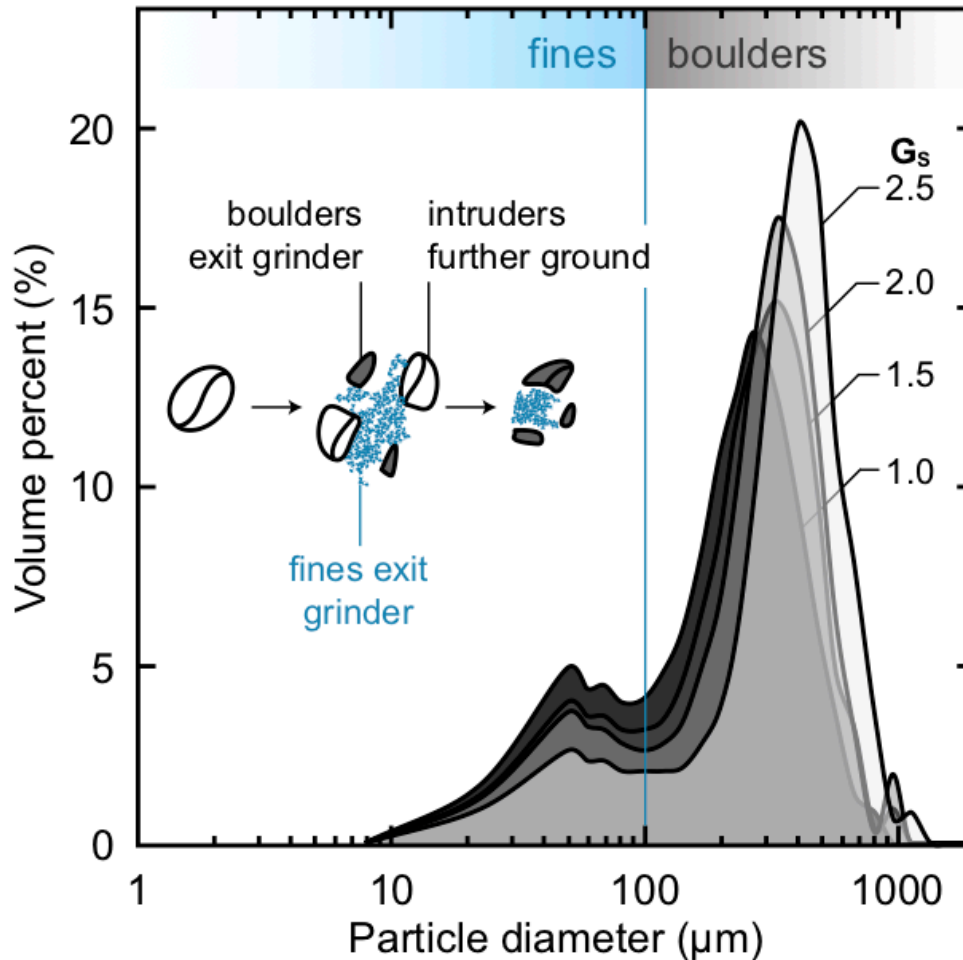




The effect of changing grind setting

Grinding finer make more fine particulates, and small large particulates

Fracturing of coffee likely proceeds through volcanic rock decomposition pathway



A theoretical explanation of grain size distributions in explosive rock fragmentation

A. C. Fowler^{1,2} and Bettina Scheu³

¹MACSI, University of Limerick, Limerick, Republic of Ireland

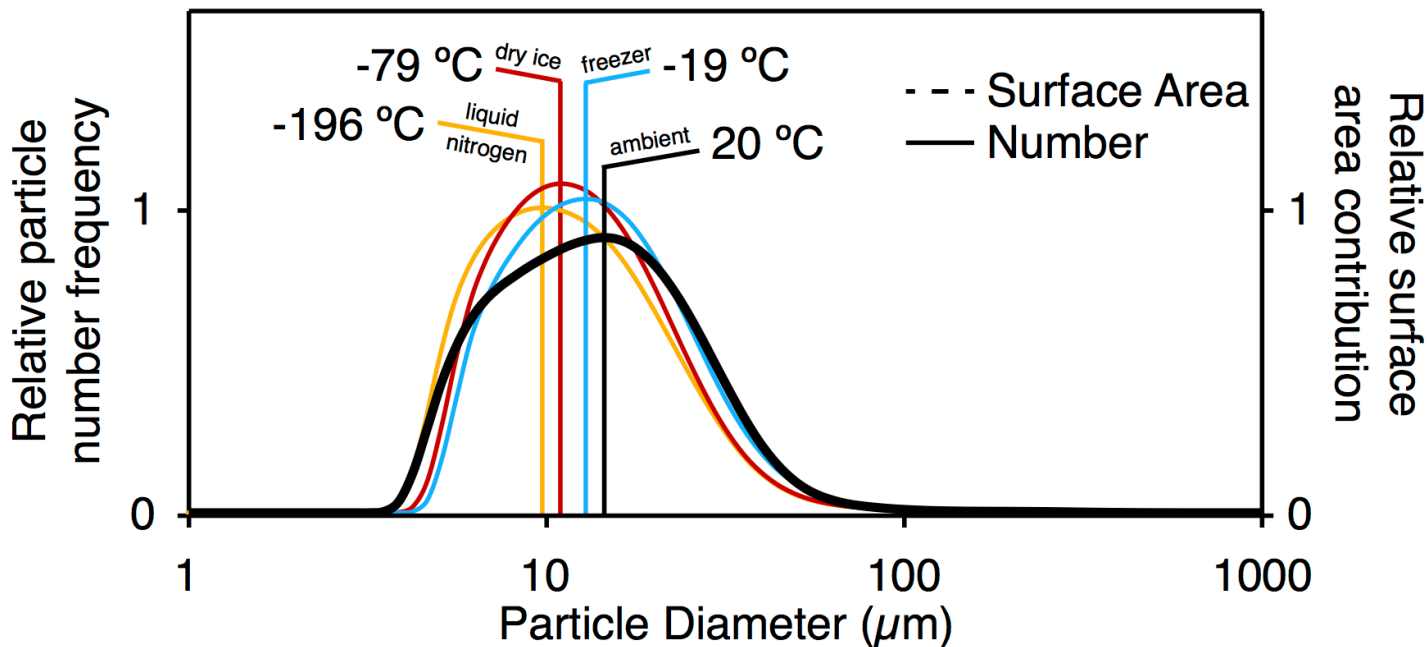
²OCIAM, University of Oxford, Oxford, UK

³Earth and Environmental Sciences, LMU München, München, Germany

ACF, 0000-0002-2062-6372

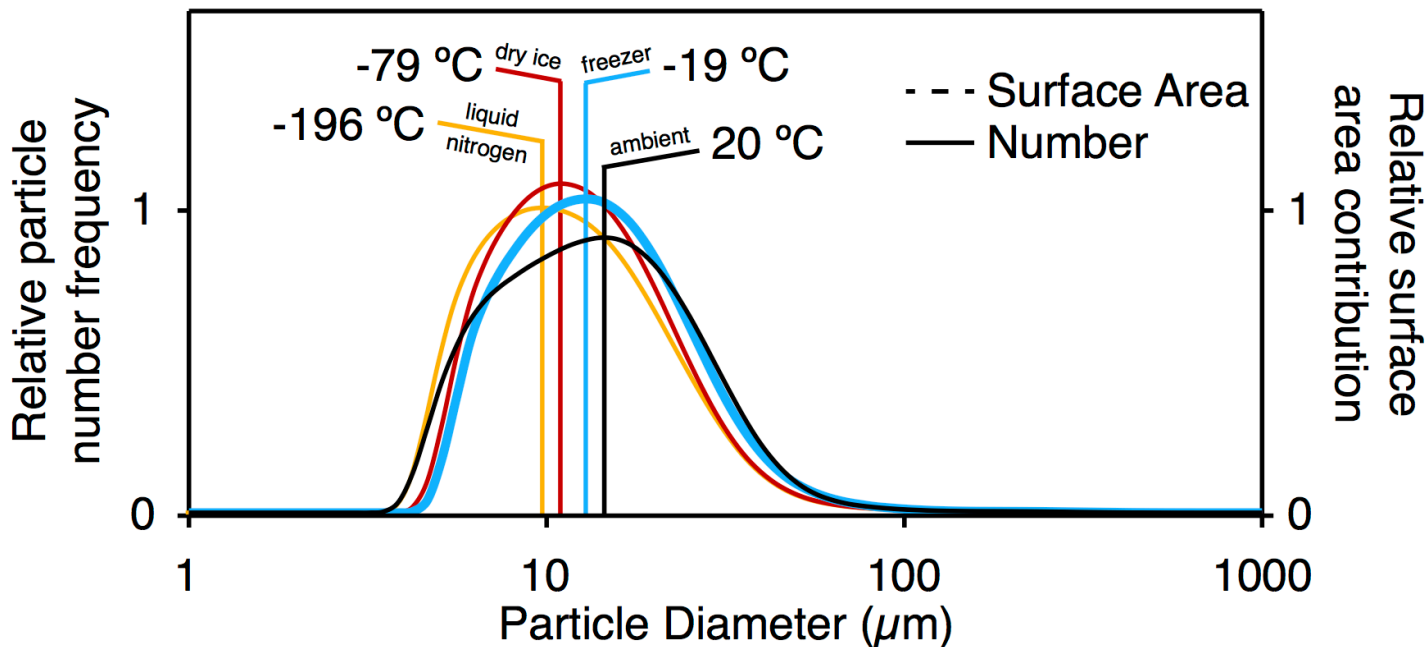


Cooling coffee before grinding augments the fine particle sizes



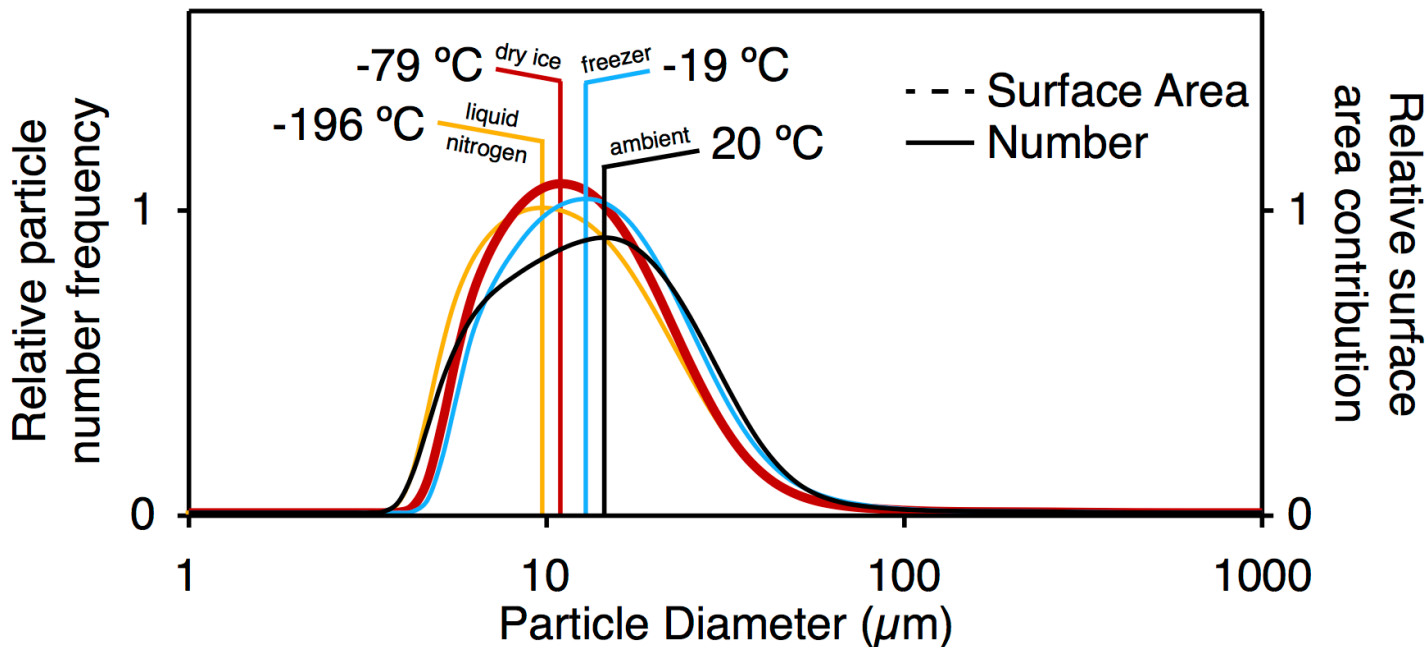


Cooling coffee before grinding augments the fine particle sizes



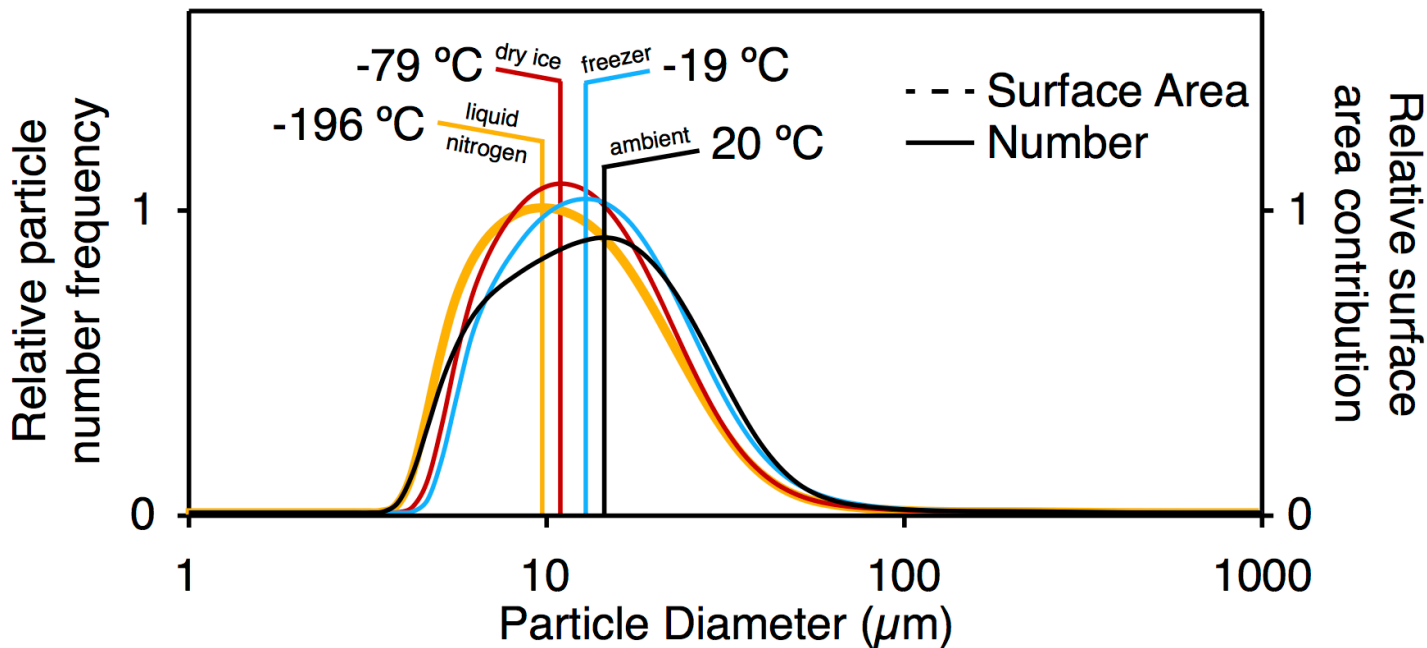


Cooling coffee before grinding augments the fine particle sizes



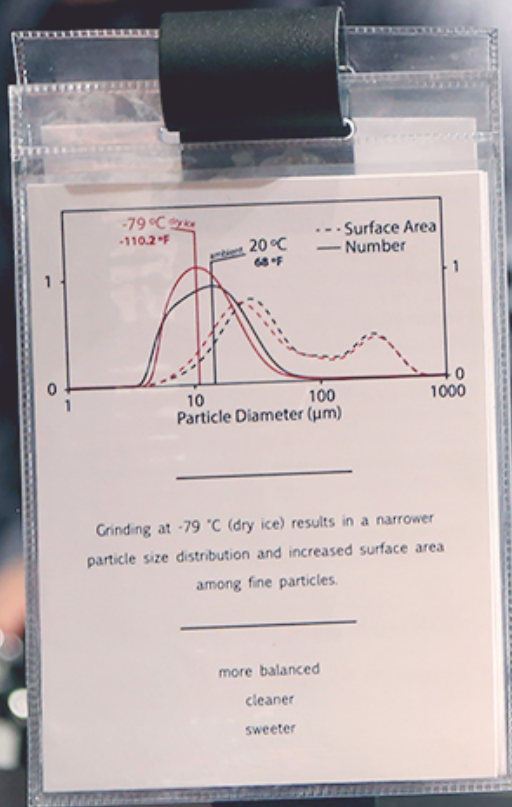


Cooling coffee before grinding augments the fine particle sizes





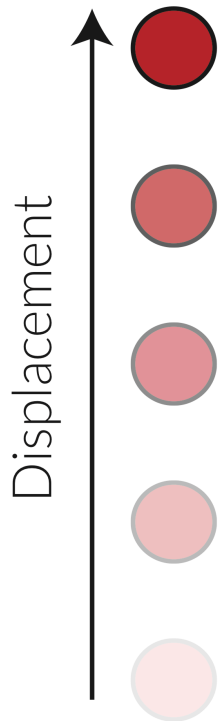
USA Barista Champion 2017 Kyle Ramage





Added benefits from cooled coffee preservation

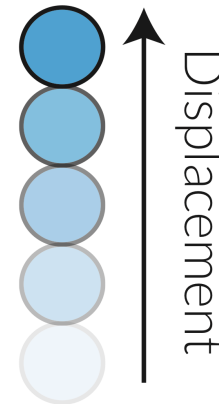
$T = 20\text{ }^{\circ}\text{C}$



from to the Arrhenius equation
(and later formalized by Eyring)

‘...the rate of a reaction doubles
for every $10\text{ }^{\circ}\text{C}$ increase in T ...’

$T = 10\text{ }^{\circ}\text{C}$





If you are going to store coffee in the fridge or freezer, store it

air tight

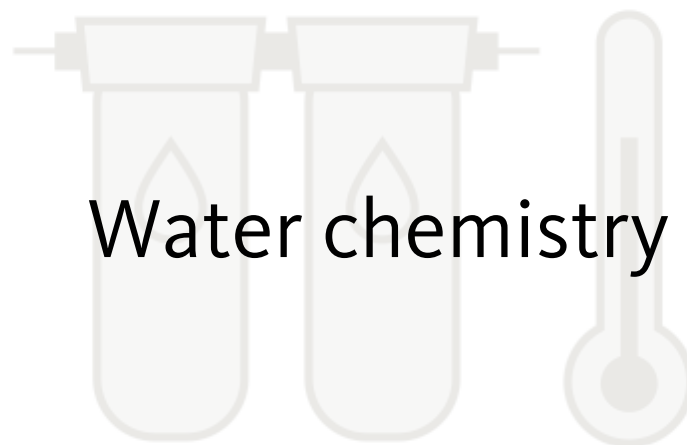
roasted coffee is extremely hygroscopic





Image courtesy of Michael Cameron



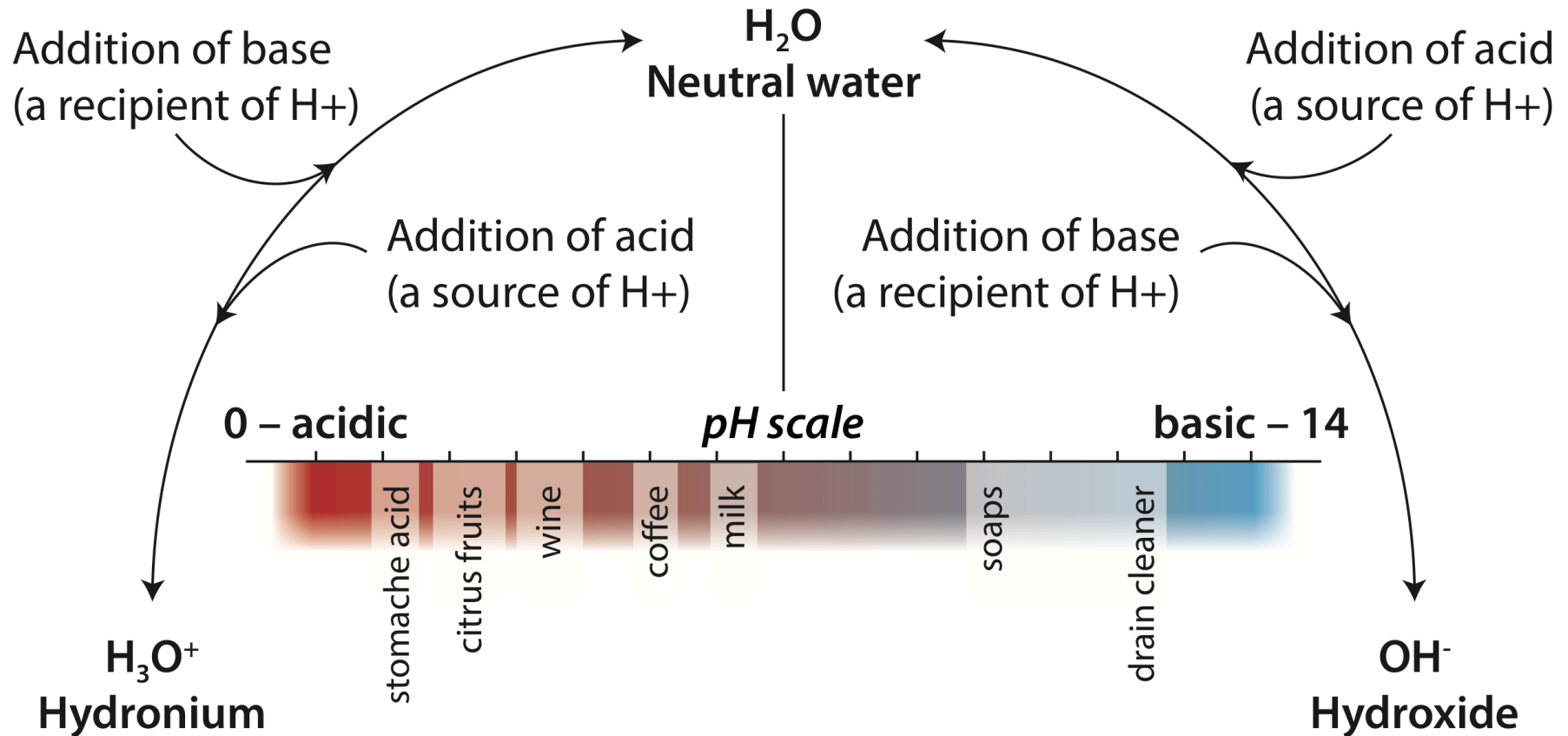


Water chemistry



The water molecule

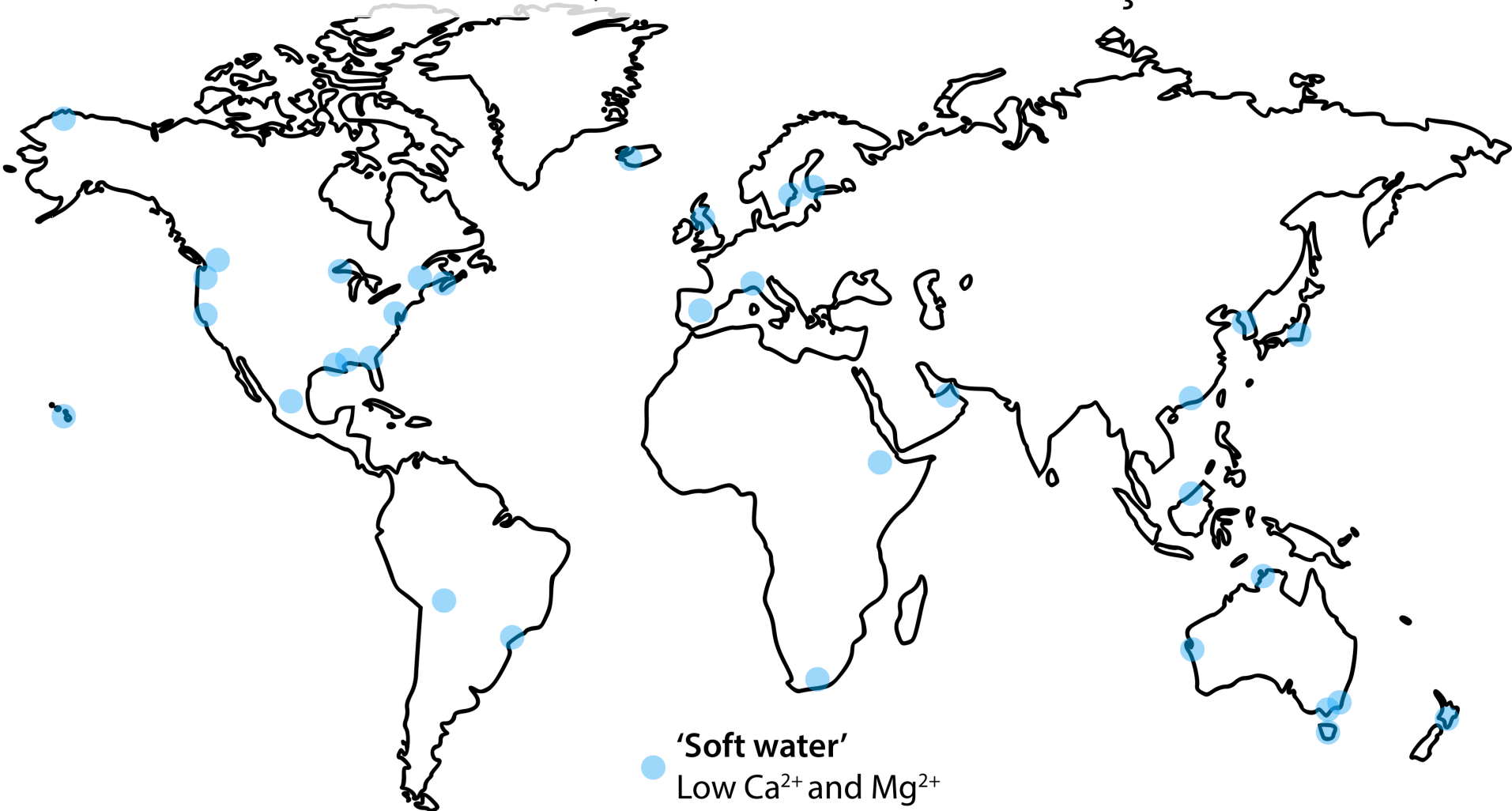
water is both an acid and a base



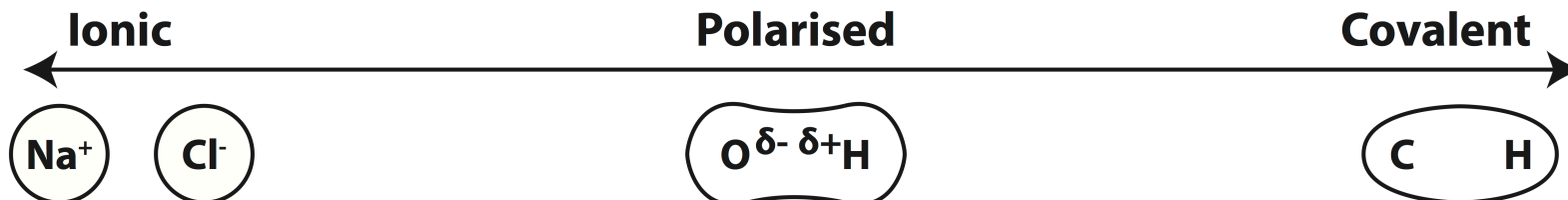


Geographical dependence on water chemistry

Soft is easier to define, hard water contains some HCO_3^- and Ca^{2+}



Atomic Number		Atomic Symbol		Atomic Name		Stable oxidation states		Electronegativity																							
1	-1,+1	H		2.20 hydrogen																											
2		He		helium																											
3	+1	Li	0.98 lithium	4	+2	Be	1.57 beryllium	5	+3	B	2.04 boron	6	-4.....+4	C	2.55 carbon	7	-3,+3 +5	N	3.04 nitrogen	8	-2	O	3.44 oxygen	9	-1	F	3.98 fluorine	10		Ne	neon
11	+1	Na	0.82 sodium	12	+2	Mg	1.31 magnesium	13	+3	Al	1.61 aluminium	14	-4,+4	Si	1.90 silicon	15	-3,+3 +5	P	2.19 phosphorus	16	-2,+2 +4 +6	S	2.58 sulfur	17	-1,+1 +3 +5 +7	Cl	3.16 chlorine	18		Ar	argon
19	+1	K	0.82 potassium	20	+2	Ca	1.00 calcium	31	+3	Ga	1.81 galium	32	-4,+2 +4	Ge	2.01 germanium	33	-3,+3 +5	As	2.18 arsenic	34	-2,+2 +4	Se	2.55 selenium	35	-1,+1 +3 +5 +7	Br	2.96 bromine	36	+2	Kr	krypton

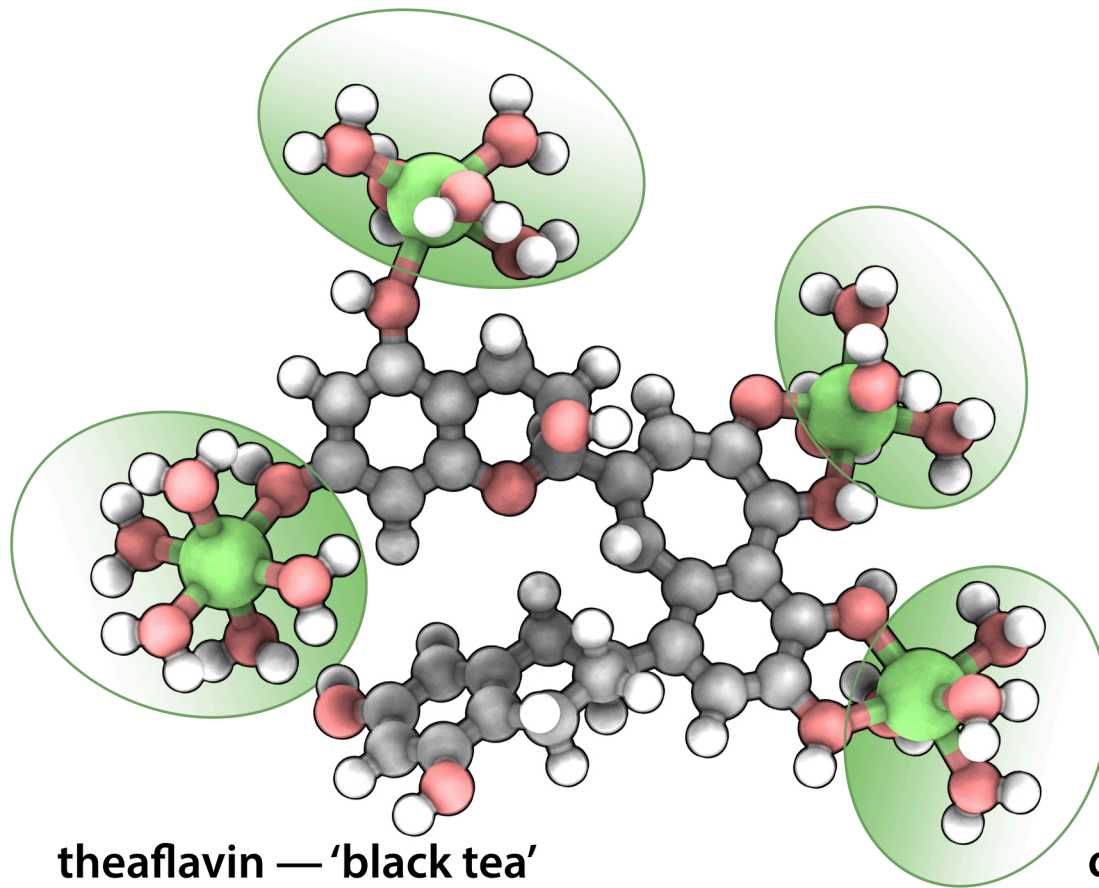


Atomic Number		Atomic Symbol		Atomic Name		Stable oxidation states		Electronegativity	
1	-1,+1	H	2.20	hydrogen					
2		He		helium					
3	+1	Li	0.98	lithium					
4	+2	Be	1.57	beryllium					
5	+3	B	2.04	boron					
6	-4.....+4	C	2.55	carbon					
7	-3,+3	N	3.04	nitrogen					
8	-2	O	3.44	oxygen					
9	-1	F	3.98	fluorine					
10		Ne		neon					
11	+1	Na	0.82	sodium					
12	+2	Mg	1.31	magnesium					
13	+3	Al	1.61	aluminium					
14	-4,+4	Si	1.90	silicon					
15	-3,+3	P	2.19	phosphorus					
16	-2,+2	S	2.58	sulfur					
17	-1,+1	Cl	3.16	chlorine					
18		Ar		argon					
19	+1	K	0.82	potassium					
20	+2	Ca	1.00	calcium					
31	+3	Ga	1.81	galium					
32	-4,+2	Ge	2.01	germanium					
33	-3,+3	As	2.18	arsenic					
34	-2,+2	Se	2.55	selenium					
35	-1,+1	Br	2.96	bromine					
36	+2	Kr		krypton					

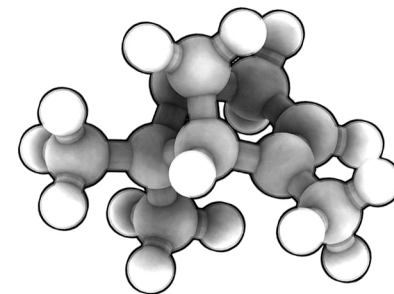
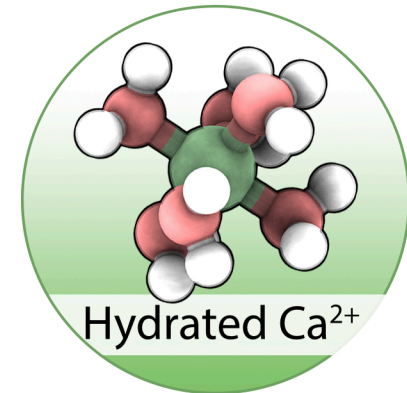


Metals binding to polar molecules

A high fidelity perspective of ionic strength



theaflavin — 'black tea'
binds to hydrated Ca^{2+}
through oxygen

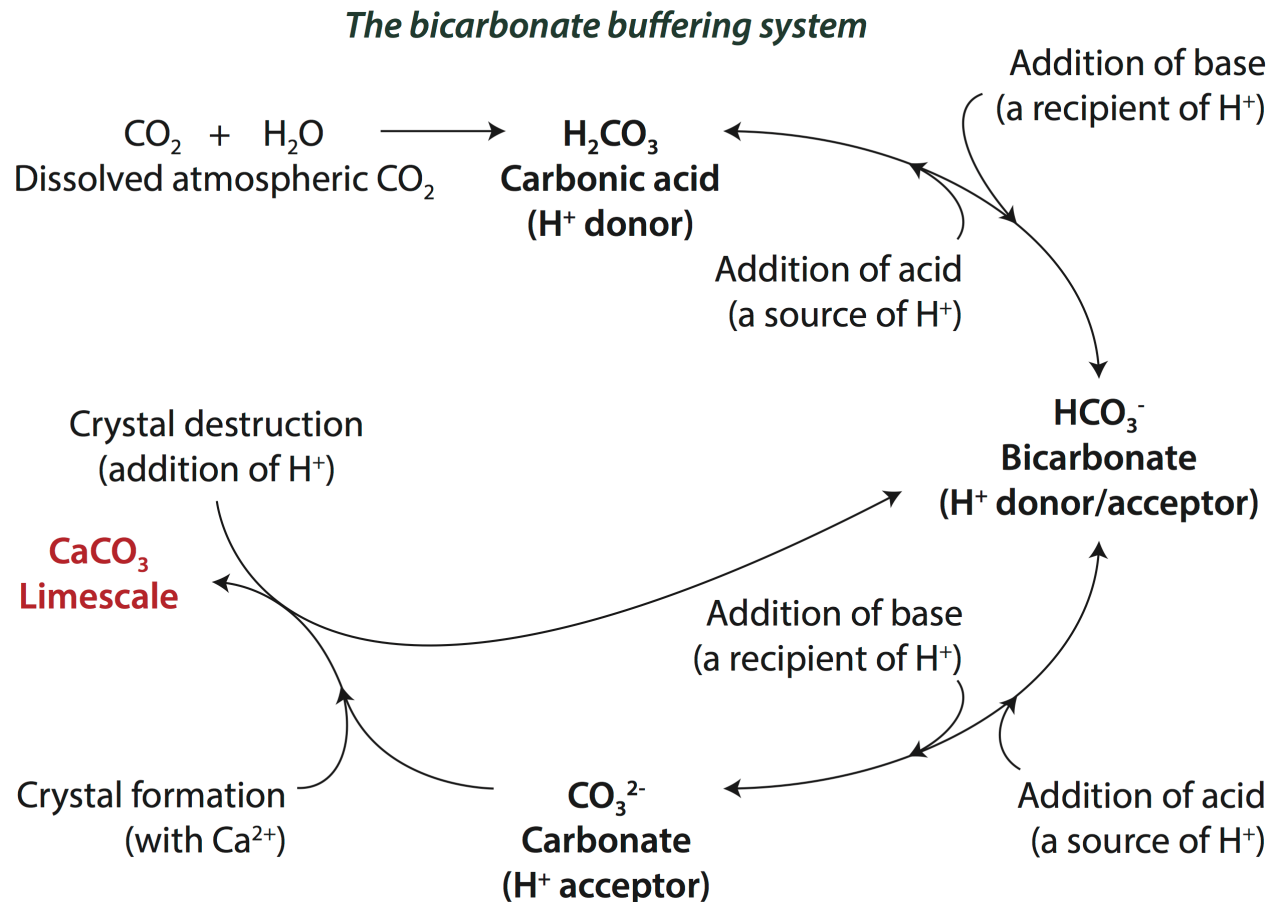


α -pinene — 'chamomile'
does not bind to Ca^{2+}
 α -pinene is non-polar



Bicarbonate (HCO_3^-)

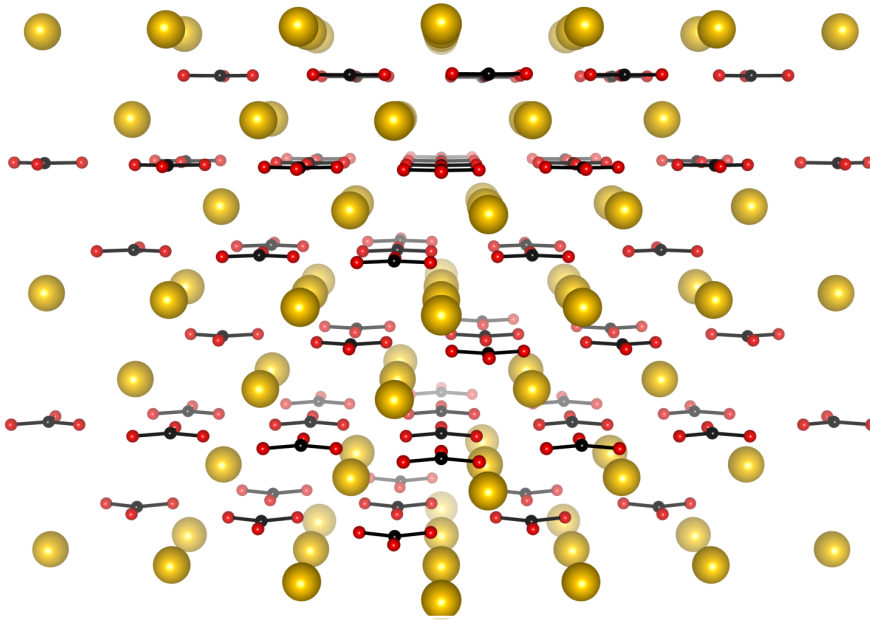
The buffer – minimizing pH fluctuations





Calcium carbonate

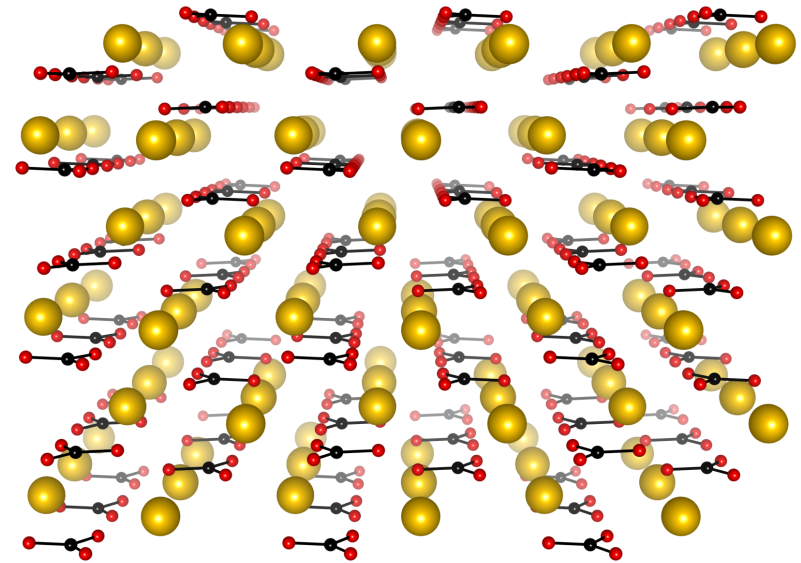
$\text{Ca}^{2+} + 2(\text{HCO}_3^-)$ to yield CaCO_3 , a white insoluble solid



Calcite

Sheet-like

Shows up on the bottom of flat kettles

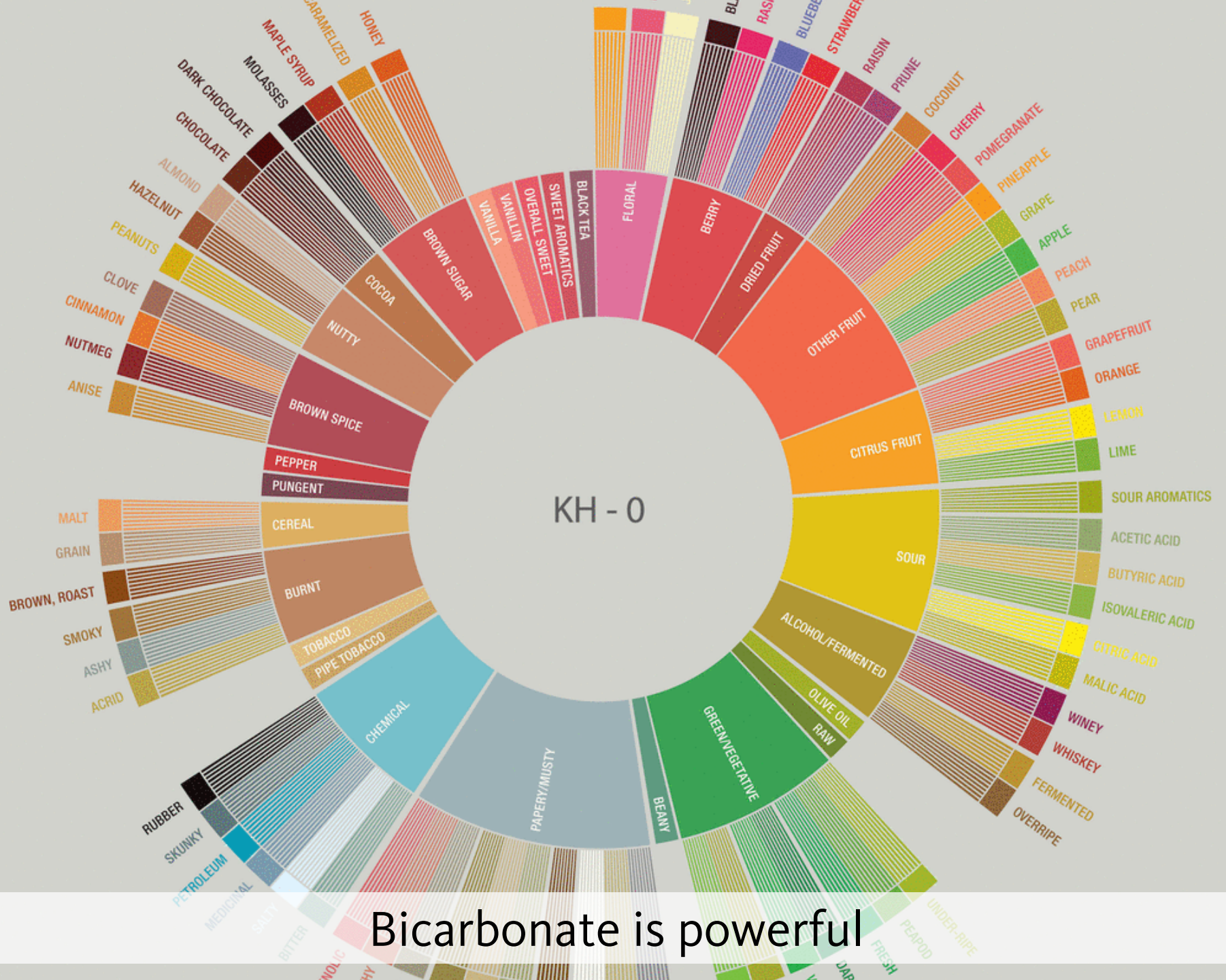


Aragonite

Jagged

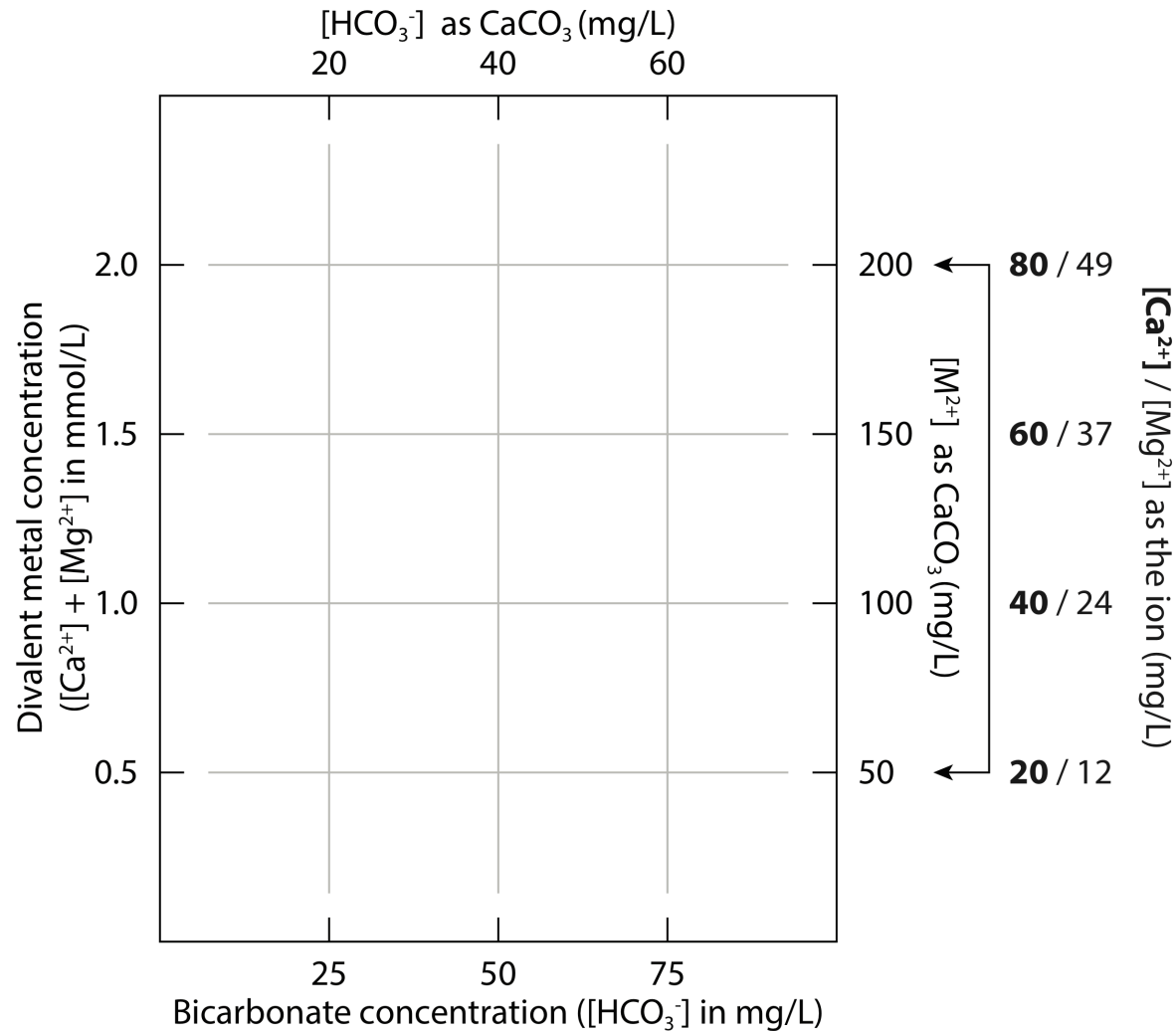
Found on the end of taps





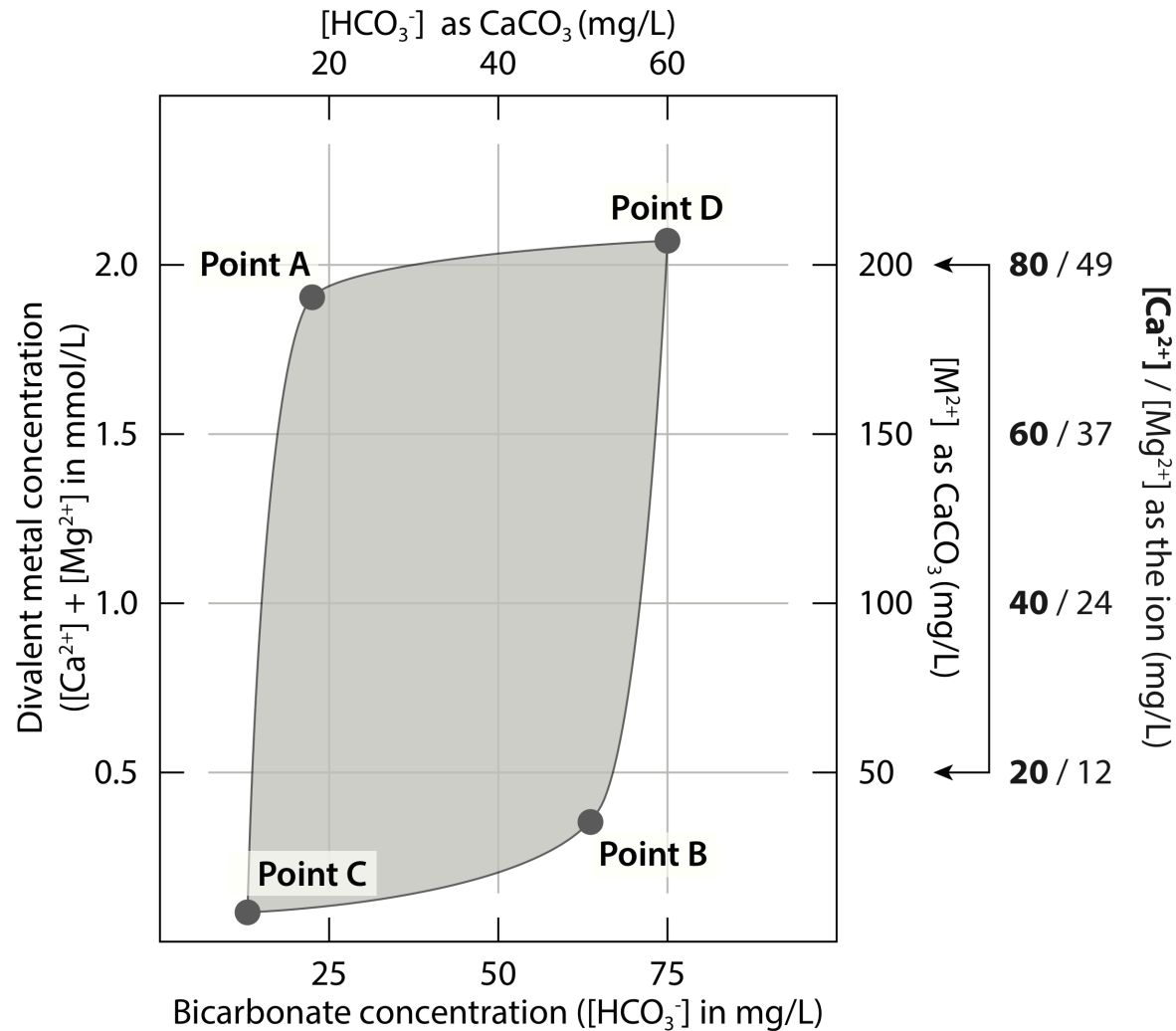
Bicarbonate is powerful

What water do we want for coffee?



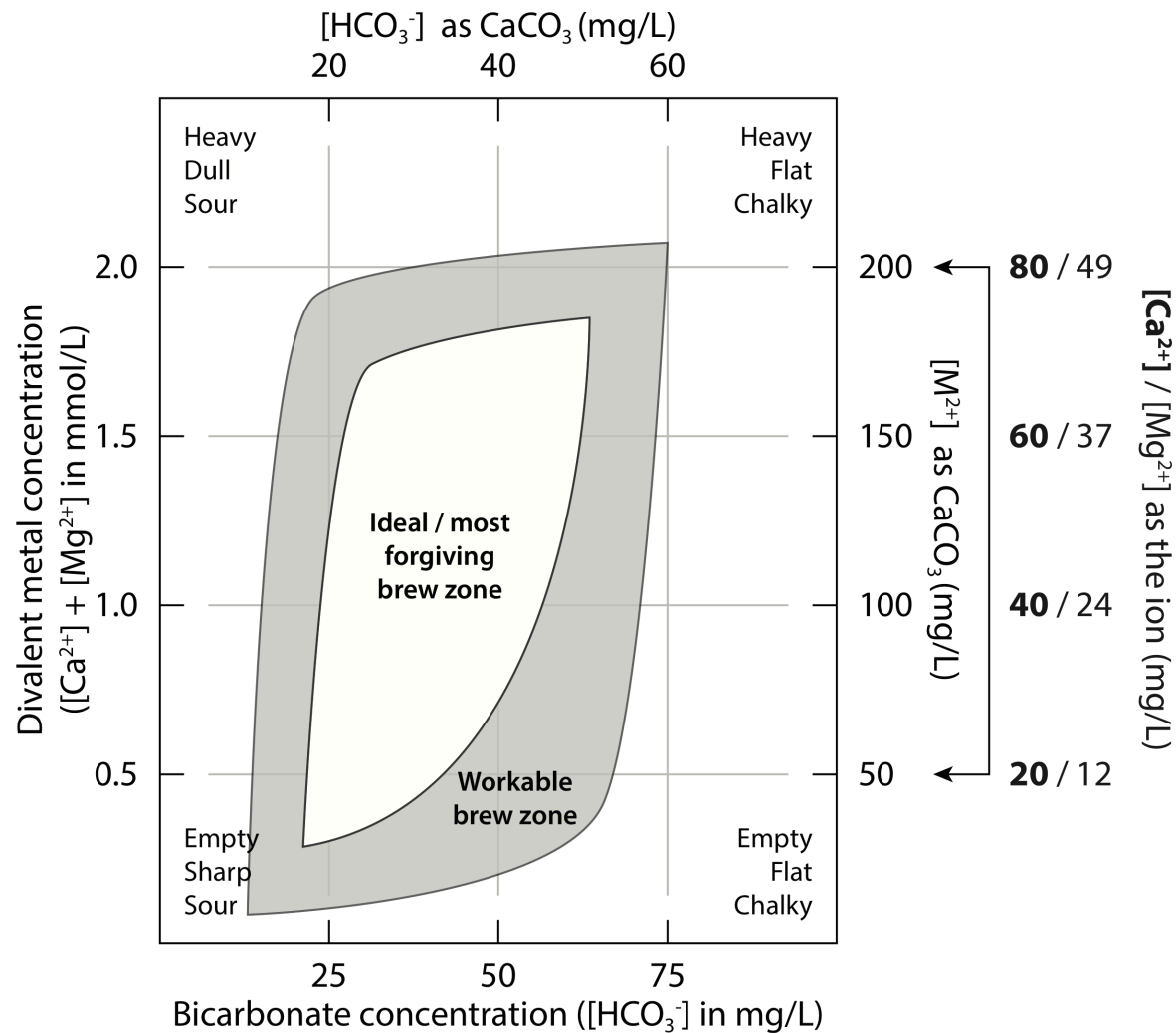


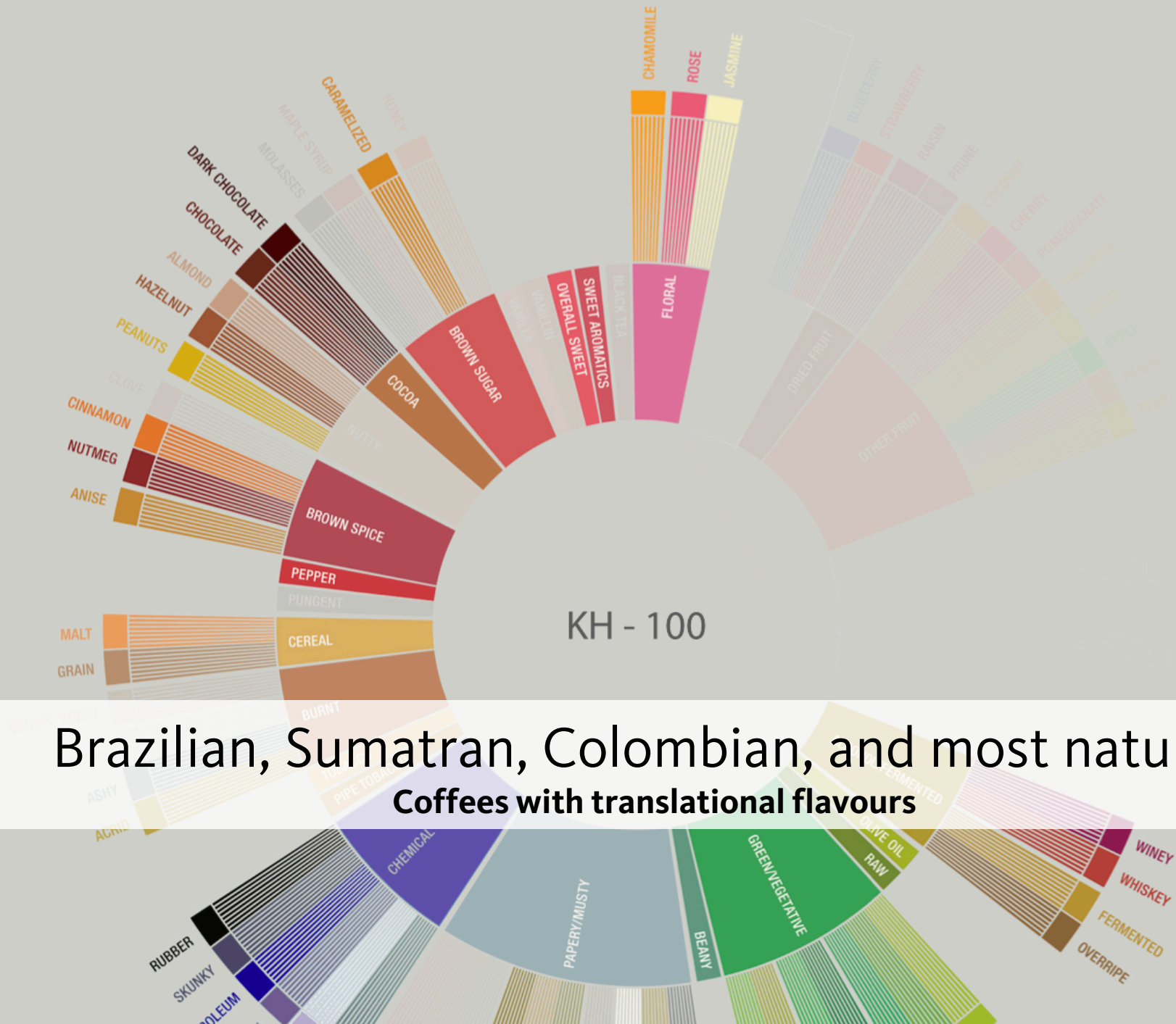
Not too much of anything





Our empirical ideal brew zone





Brazilian, Sumatran, Colombian, and most naturals
Coffees with translational flavours

Valser Silent Swiss Water

Terrible for coffee brewing.

Auf 1'806 m Höhe entspringt rein,
quellfrisch und kristallklar das stille
Valser Silence mit dem angenehm sanften

Geschmack. *La Valser Silence naturelle au goût agréablement délicat jaillit
pure et fraîche de notre source alpine à 1'806 m d'altitude.*

**Natürliches Mineralwasser ohne Kohlensäure. Mit geringem Gehalt an
Mineralien.** Natriumarm. Totalmineralisation: 220 mg/L, davon Ca^{2+} 51, Mg^{2+} 14,
 Na^+ 0.3, HCO_3^- 153, SO_4^{2-} 8.5 mg/L. pH 7.5. Amtlich anerkannte Analyse vom 5.1.2010.
St. Paulsquelle. Kühl und trocken lagern, geschützt vor Sonnenlicht, starken Düften sowie
Chemikalien. Mindestens haltbar bis: siehe Etikette. Mehrwegflasche. Pfand CHF 0.50.
Valser Mineralquellen GmbH, CH-7132 Vals. 0848 10 20 20. | valser.ch



The Roman Baths were really hard

SPA WATER ANALYSIS

Minerals present in milligrams per litre (2012 analysis)

Sulphate (SO ₄)	891.0000
Calcium (Ca)	406.4000
Chloride (Cl)	333.6000
Sodium (Na)	205.0000
Bicarbonate (HCO ₃)	151.0000
Magnesium (Mg)	53.7000
Silica (SiO ₂)	21.4200
Potassium (K)	17.5000
Strontium (Sr)	6.6000
Fluoride* (F)	3.2500
Bromide (Br)	1.9300
Iron (Fe)	0.8000



Some handy water recipes

for better or worse

The front and center

0.25 g/L $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ (epsom salt)

~25 ppm Mg^{2+} as Mg^{2+}

0.05 g/L NaHCO_3 (baking soda)

~35 ppm HCO_3^- as HCO_3^-

The 7 n' 7

0.3 g/L $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ (gypsum salt)

~70 ppm Ca^{2+} as Ca^{2+}

0.11 g/L NaHCO_3 (baking soda)

~70 ppm HCO_3^- as HCO_3^-

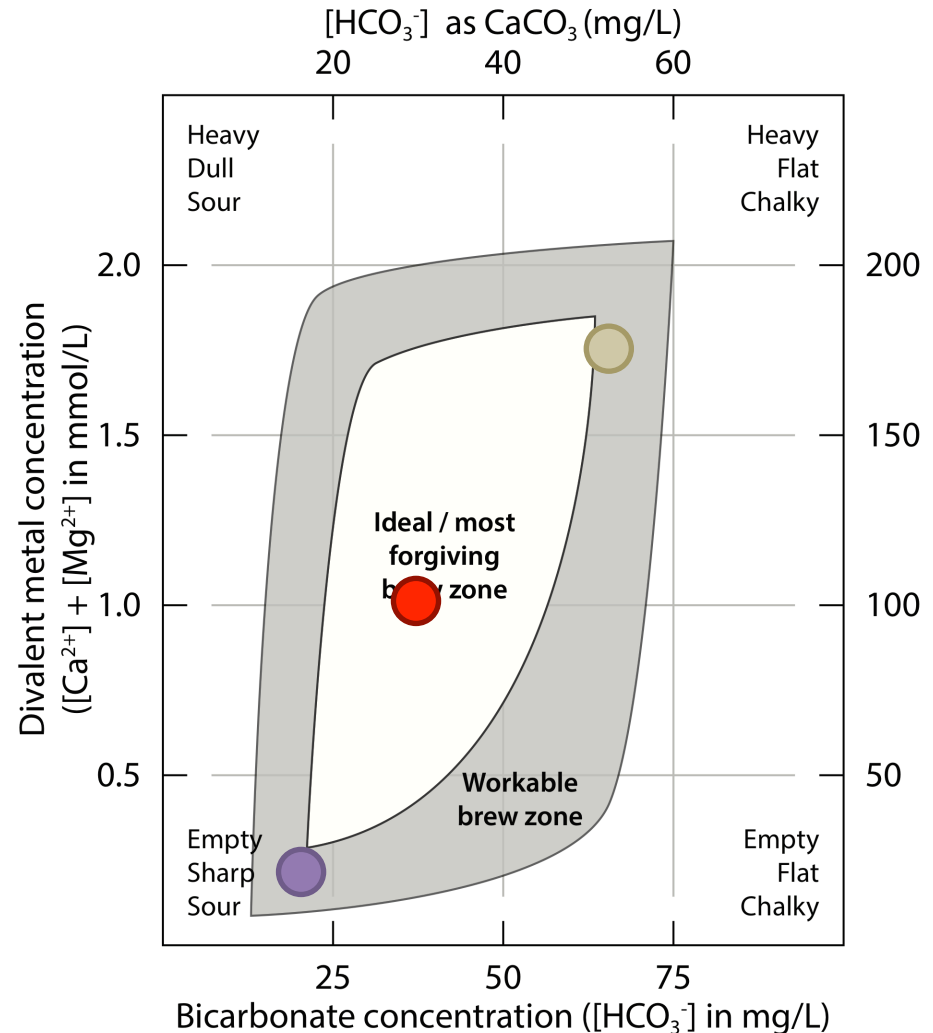
The double rizzi banger

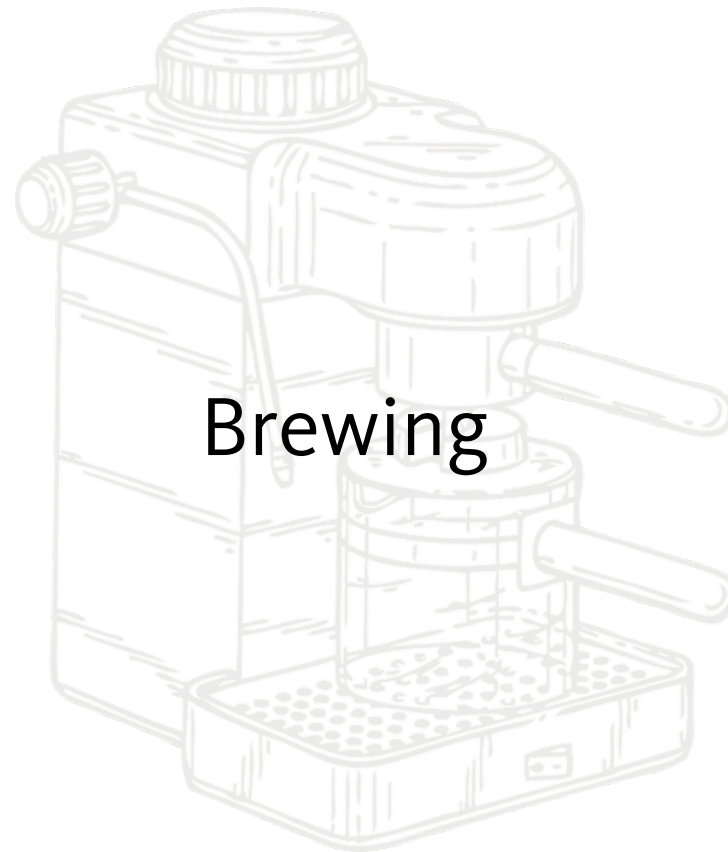
0.05 g/L $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ (gypsum salt)

~5 ppm Mg^{2+} as Mg^{2+}

0.02 g/L NaHCO_3 (baking soda)

~15 ppm HCO_3^- as HCO_3^-





Brewing

What do you need to prepare espresso and do experimental coffee science?



\$1,000 - \$40,000



The definition of *espresso*

The Specialty Coffee Association (SCA) defines espresso as “a **25-35mL** beverage prepared from **7-9 grams of coffee** through which clean water of 195°- 205 °F (**92°-95°C**) has been forced at **9-10 atmospheres of pressure**, and where the grind of the coffee is such that the brewing ‘flow’ time is approximately **20-30 seconds.**”



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7 g vs. 20 g baskets



The definition of *espresso*

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Nobody makes espresso anymore



Time: The one gospel

The Specialty Coffee Association (SCA) defines espresso as “a **25-35mL** beverage prepared from **7-9 grams of coffee** through which clean water of 195°- 205 °F (**92°-95°C**) has been forced at **9-10 atmospheres of pressure**, and where the grind of the coffee is such that the brewing ‘flow’ time is approximately

20-30 seconds.”

Espresso machines have been used for conventional chemical applications



Letter

pubs.acs.org/OrgLett

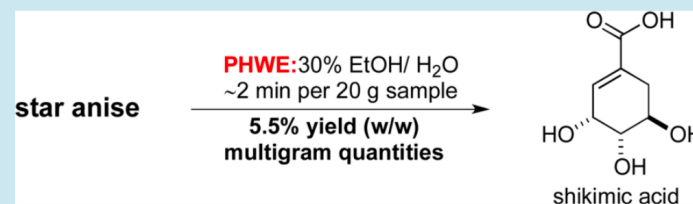
New Method for the Rapid Extraction of Natural Products: Efficient Isolation of Shikimic Acid from Star Anise

Jeremy Just,[†] Bianca J. Deans,[†] Wesley J. Olivier,[†] Brett Paull,^{†,‡} Alex C. Bissember,^{*,†} and Jason A. Smith^{*,†}

[†]School of Physical Sciences – Chemistry and [‡]Australian Centre for Research on Separation Science (ACROSS), University of Tasmania, Hobart, Tasmania 7001, Australia

Supporting Information

ABSTRACT: A new, practical, rapid, and high-yielding process for the pressurized hot water extraction (PHWE) of multigram quantities of shikimic acid from star anise (*Illicium verum*) using an unmodified household espresso machine has been developed. This operationally simple and inexpensive method enables the efficient and straightforward isolation of shikimic acid and the facile preparation of a range of its synthetic derivatives.





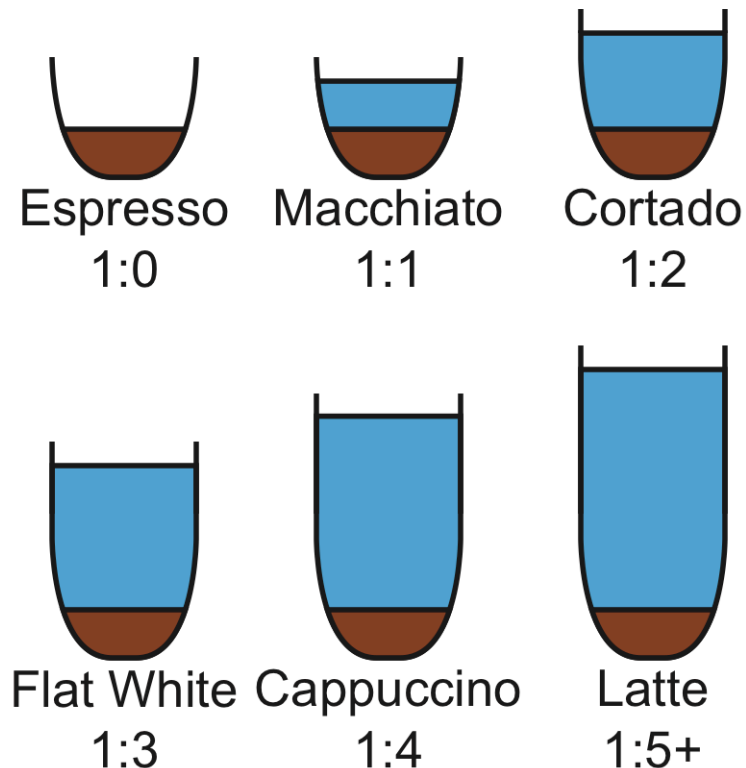
Espresso machines have been used for conventional chemical applications



Figure S1: Extraction of star anise using an espresso machine.



The modern espresso menu

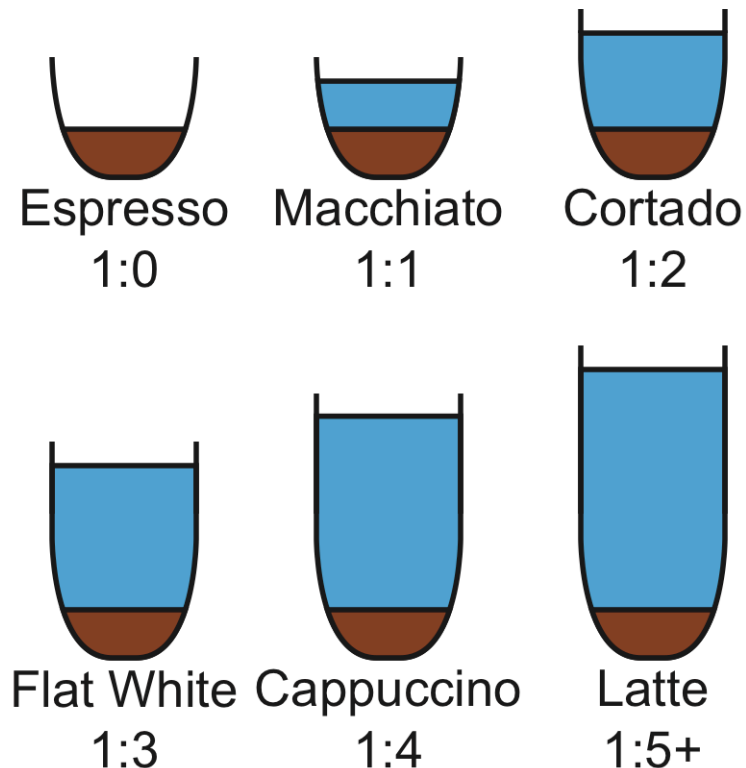


Espresso is a drink prepared with an espresso machine, and typically features about **10% coffee mass per mass of liquid**

Implication: The volume/mass of the espresso determines the volume/mass of milk required to achieve drink definition.



The Australian's ruined everything

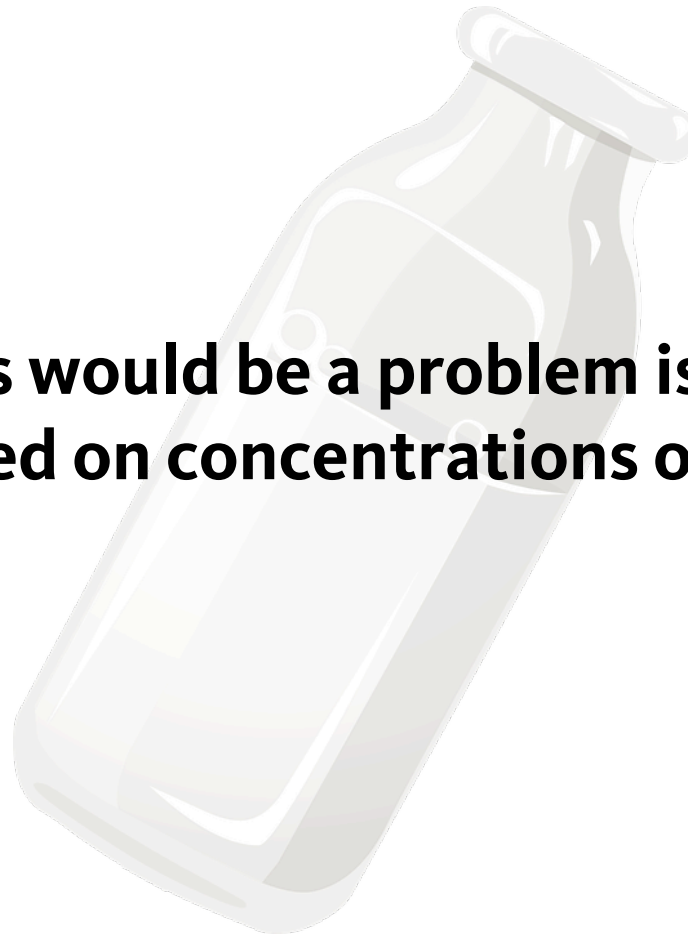


A single espresso is half of the volume and physical shot produced when a 20 g basket is used.

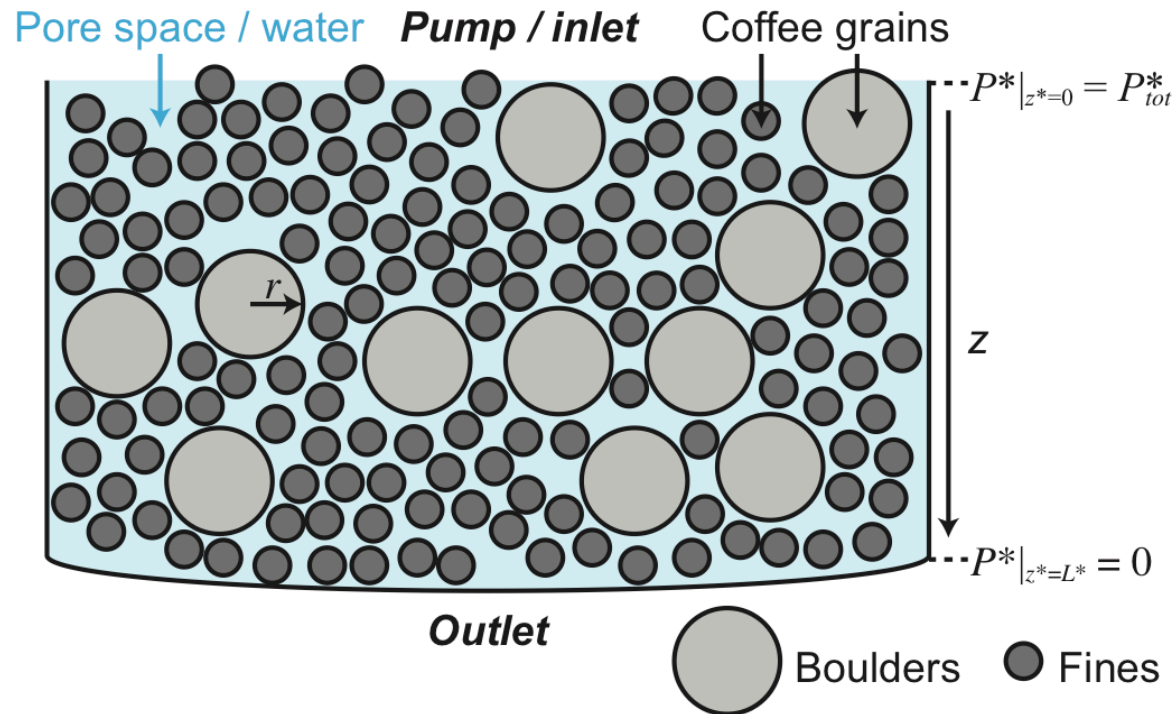
A double espresso is the entire liquid produced in a single extraction.



None of this would be a problem if we all made beverages based on concentrations of coffee in milk.



Development of a numerical model for extraction from a granular bed

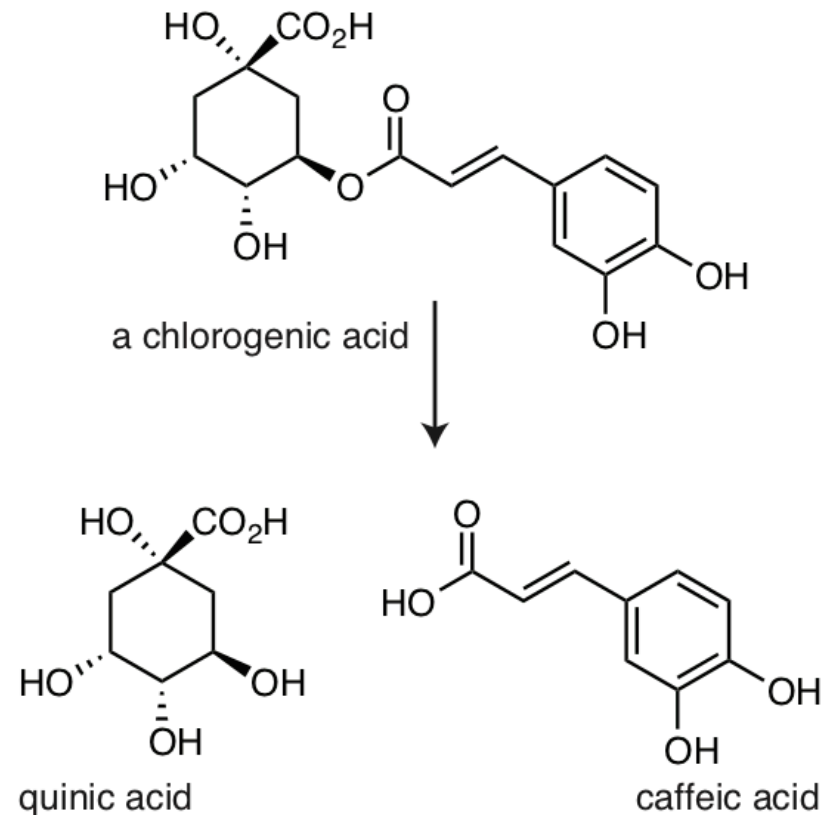
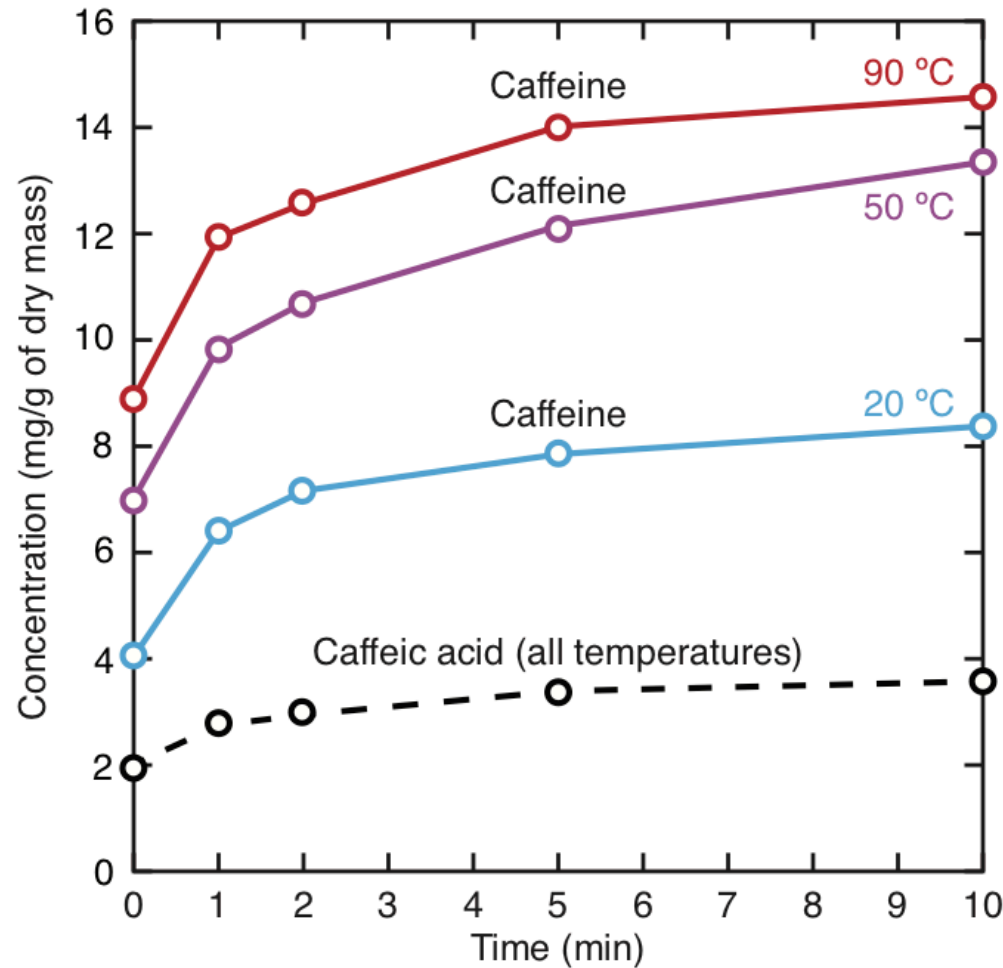


Ω_s – the volume fraction occupied by coffee grains

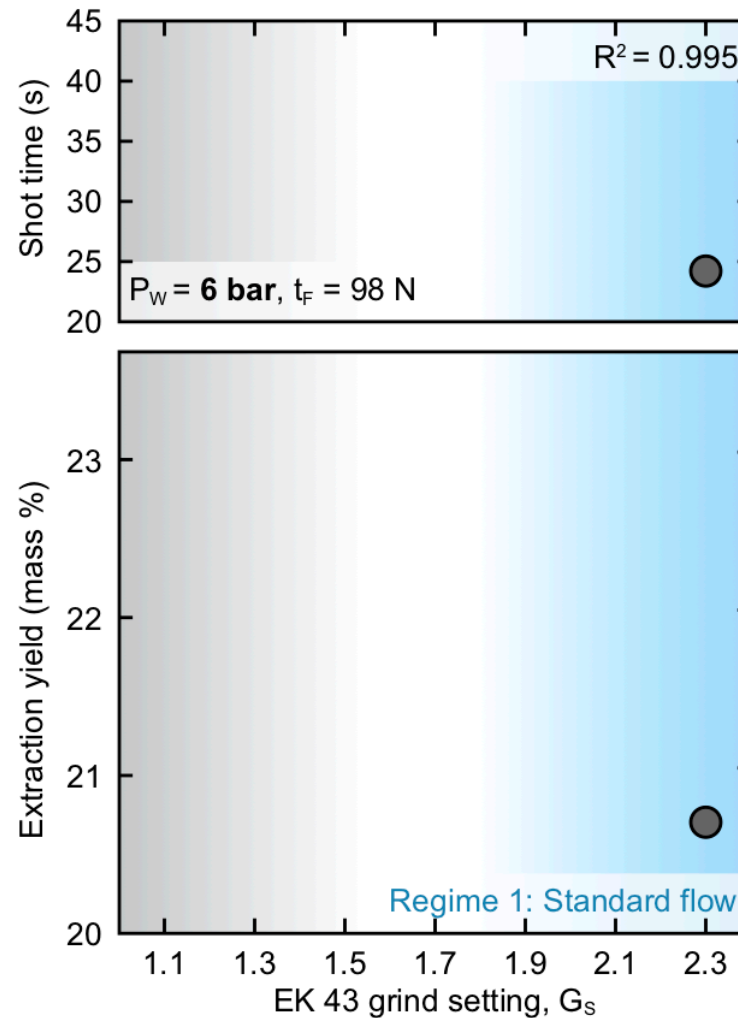
Ω_L – the volume fraction occupied by liquid

Experimental kinetics

isolating temperature and molecular dissolution rates

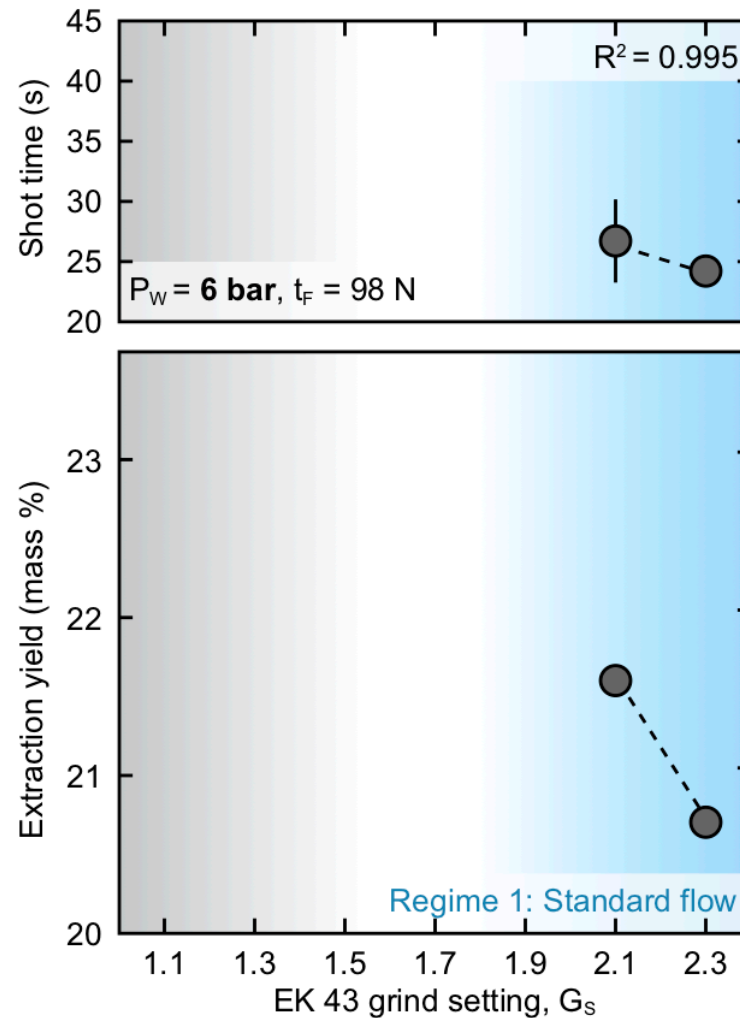


The curious problem of grinding finer



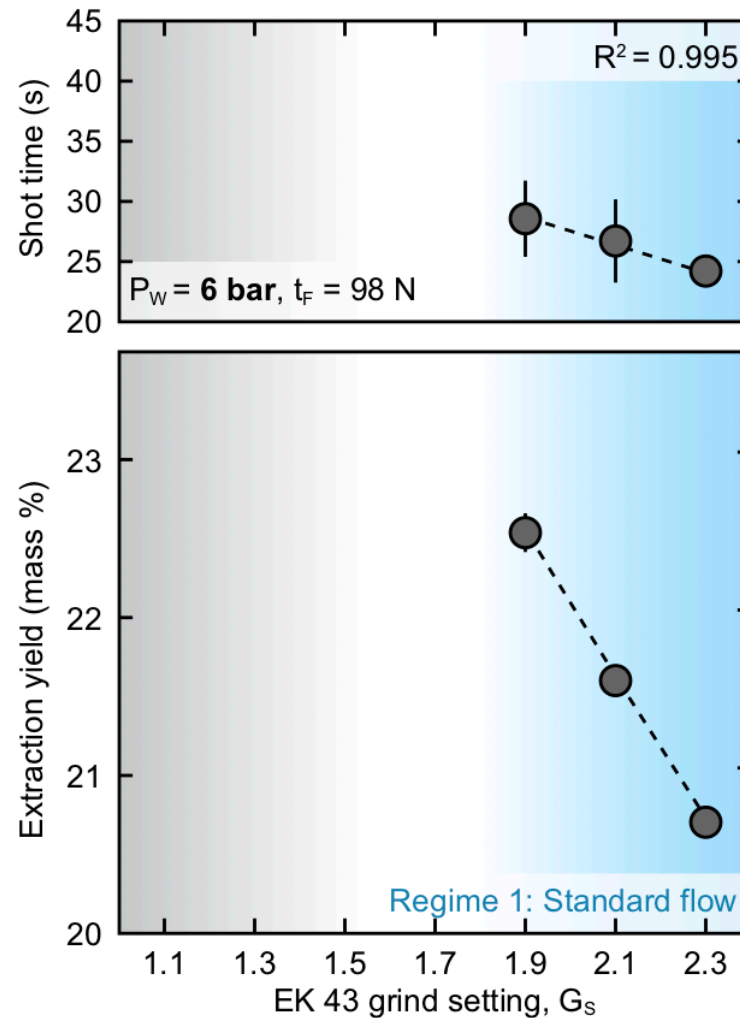


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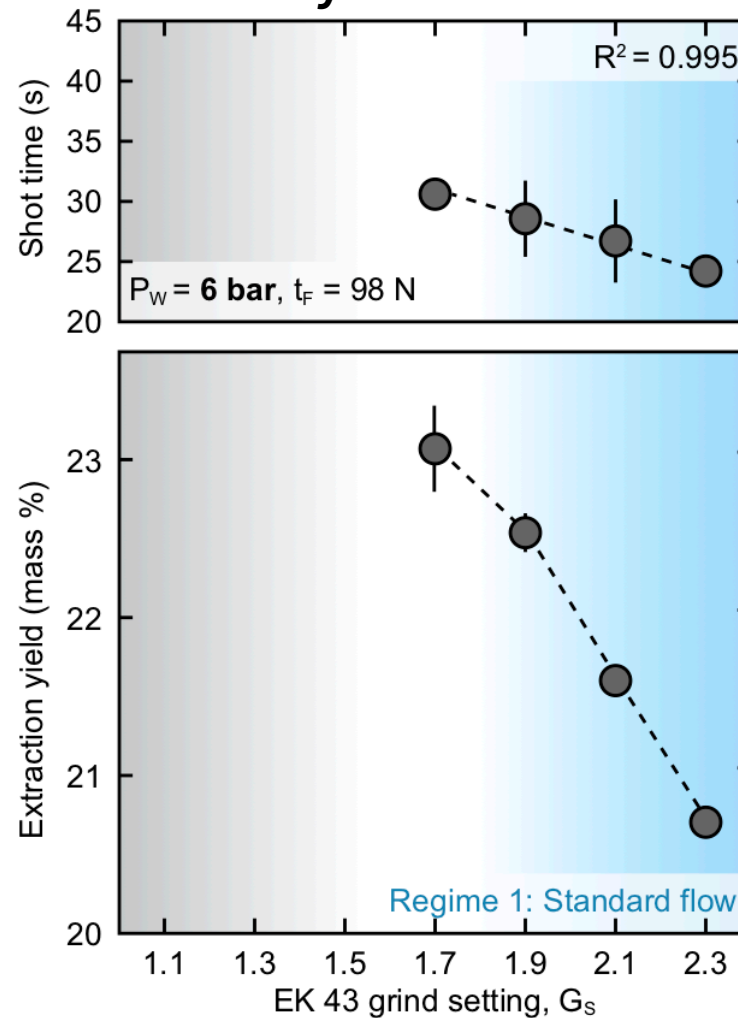


The curious problem of grinding finer



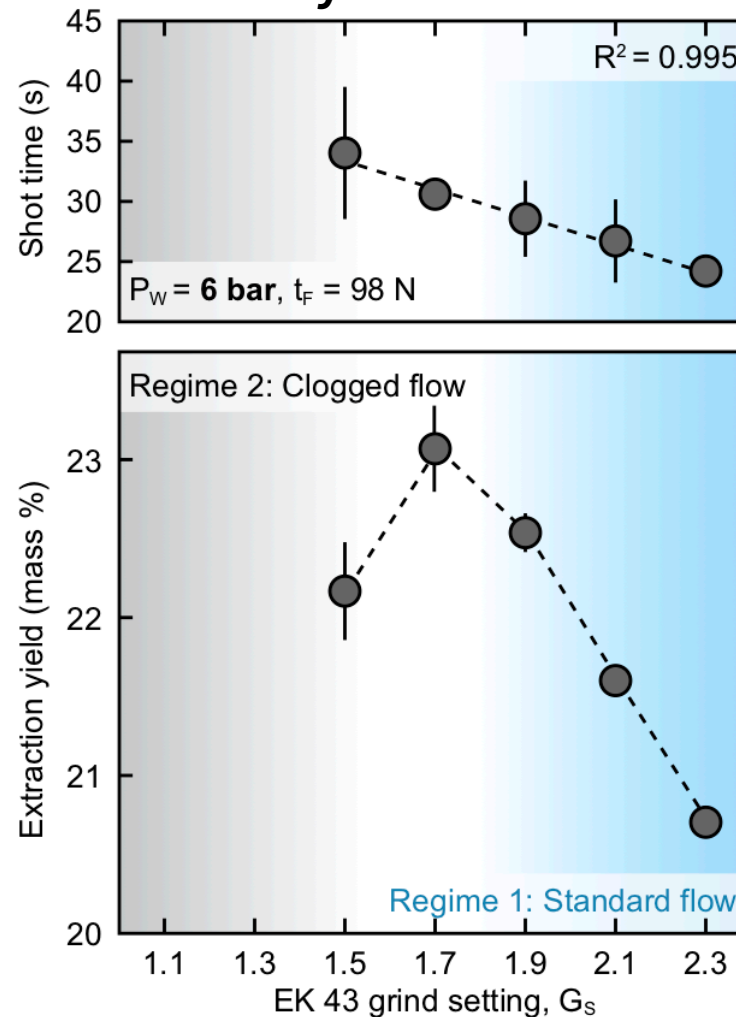
The curious problem of grinding finer

The key observation



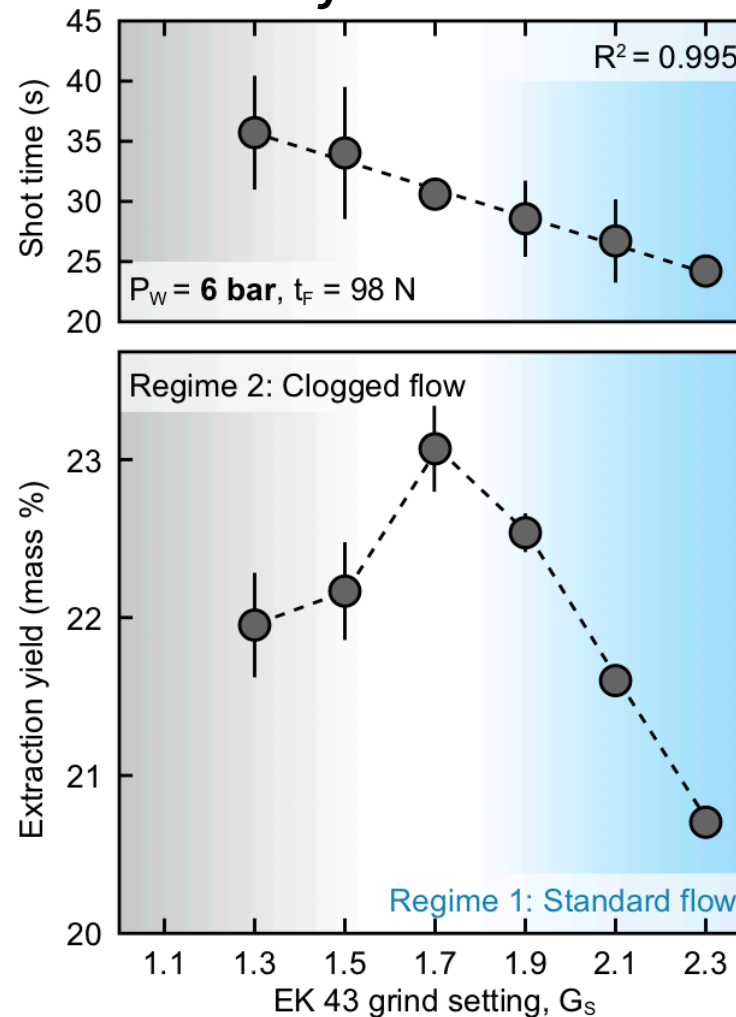
The curious problem of grinding finer

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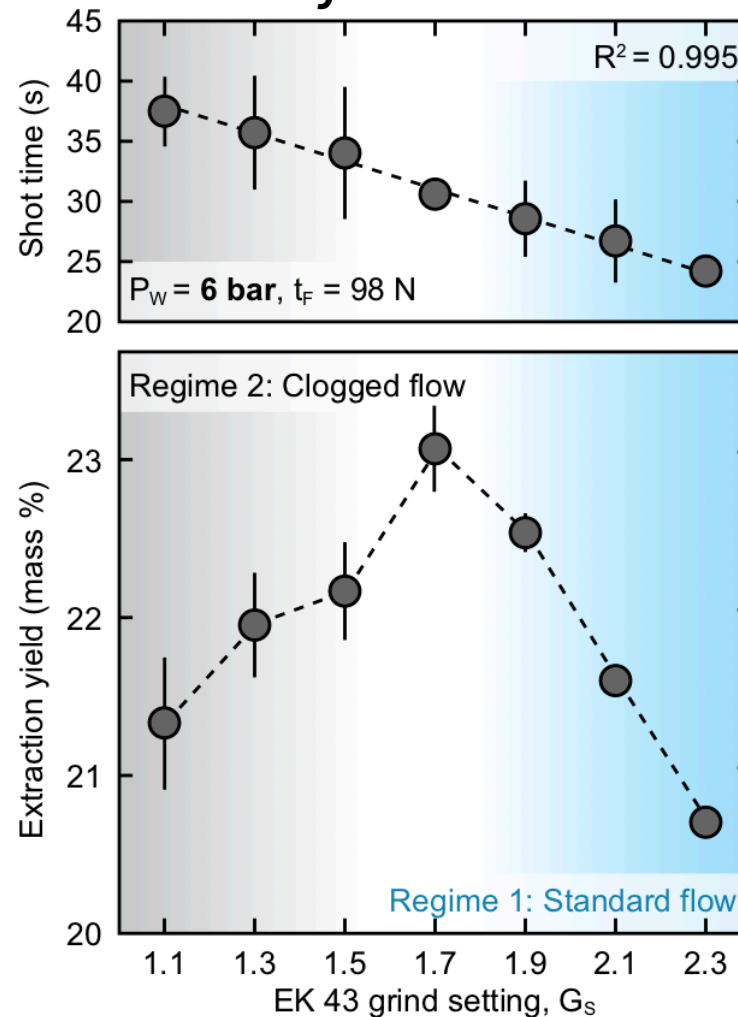
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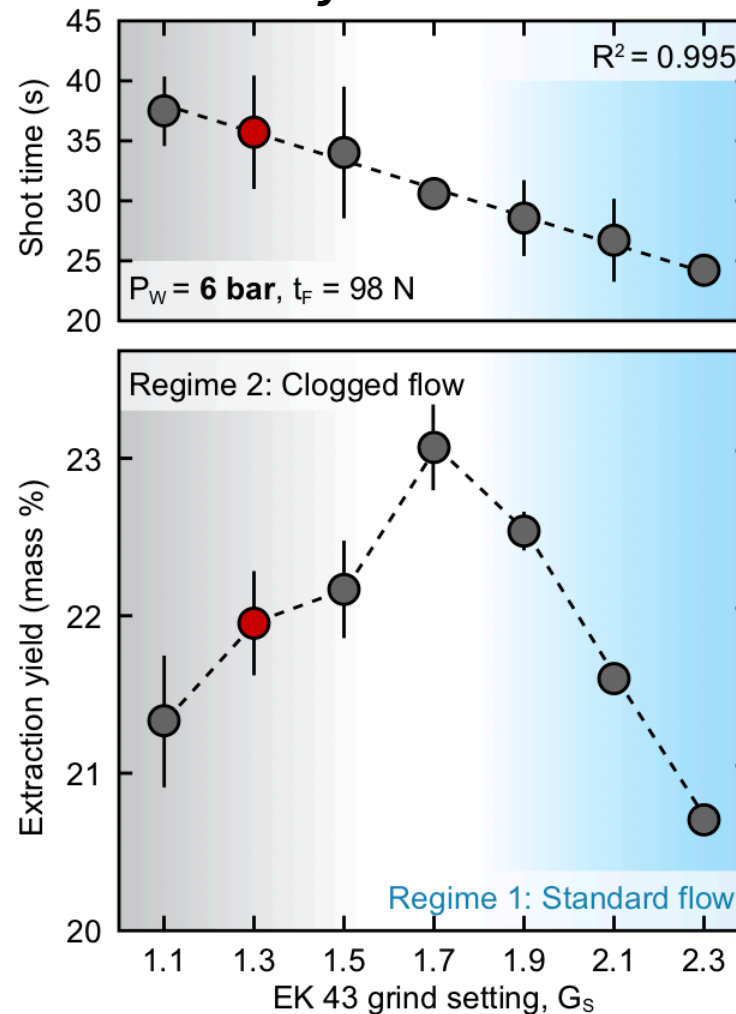
The curious problem of grinding finer

The key observation



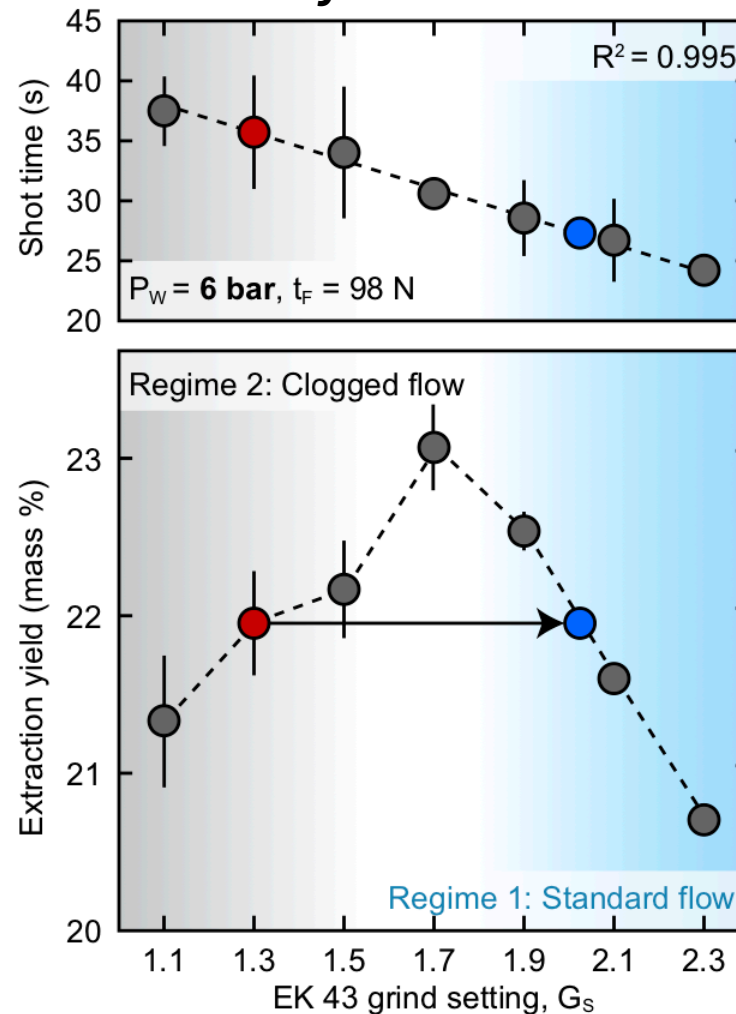
The curious problem of grinding finer

The key observation



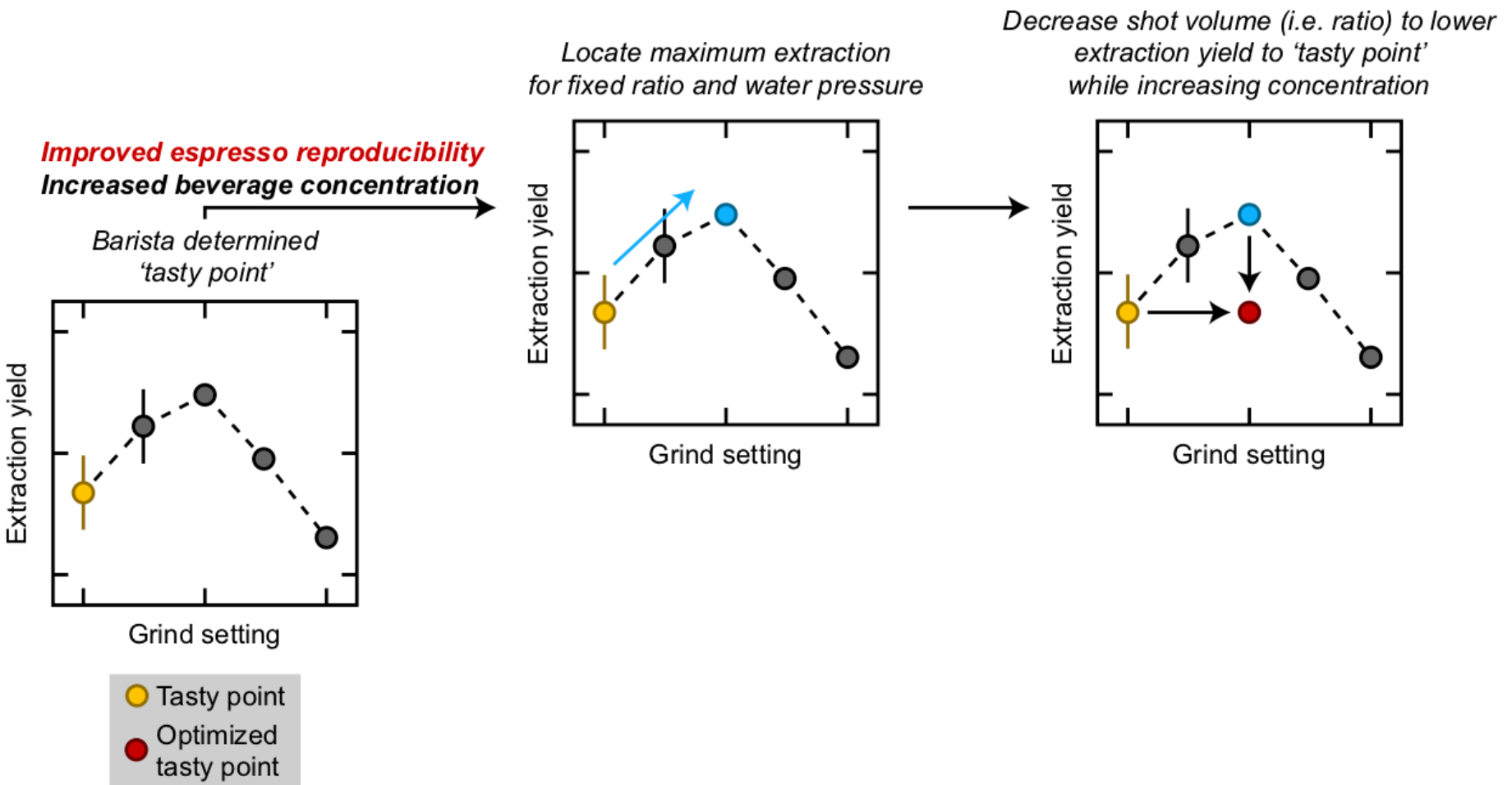
The curious problem of grinding finer

The key observation



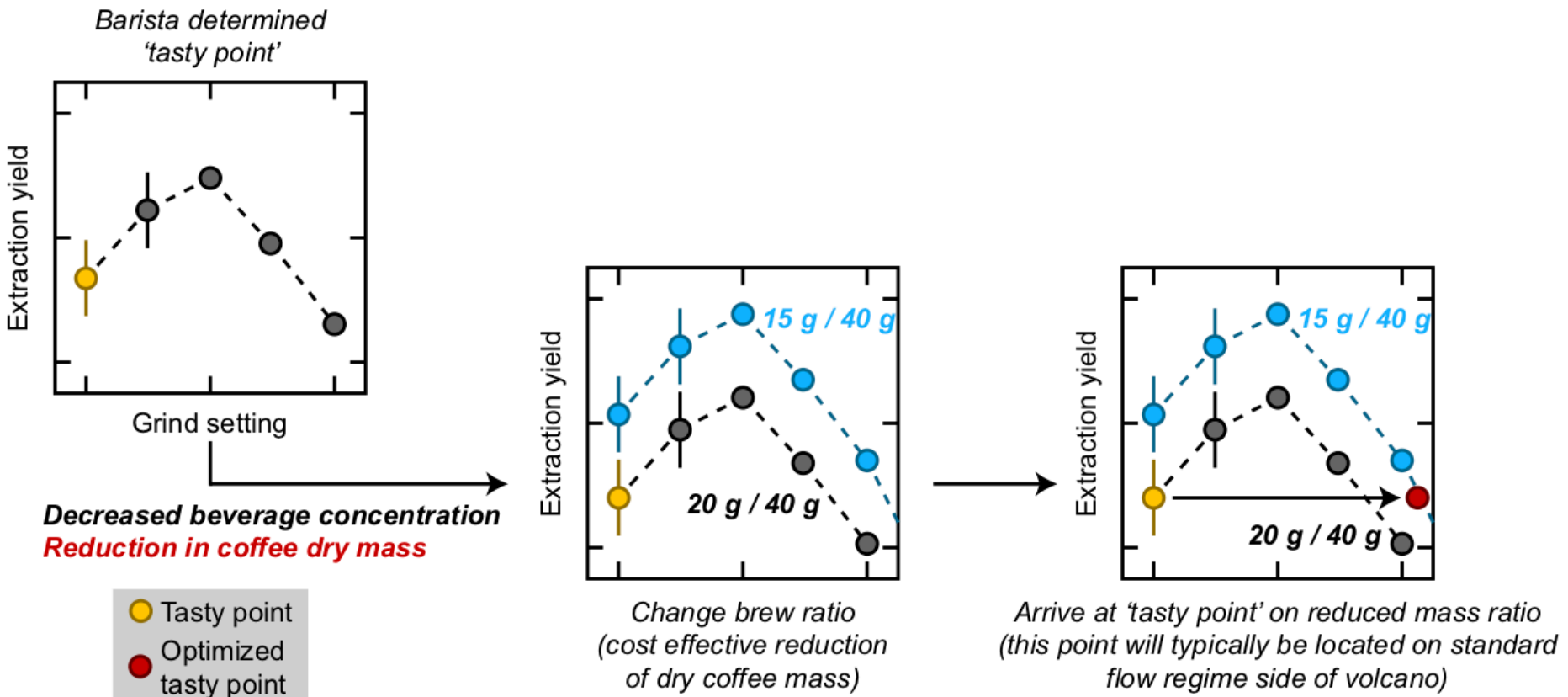


Optimizing espresso for reproducibility



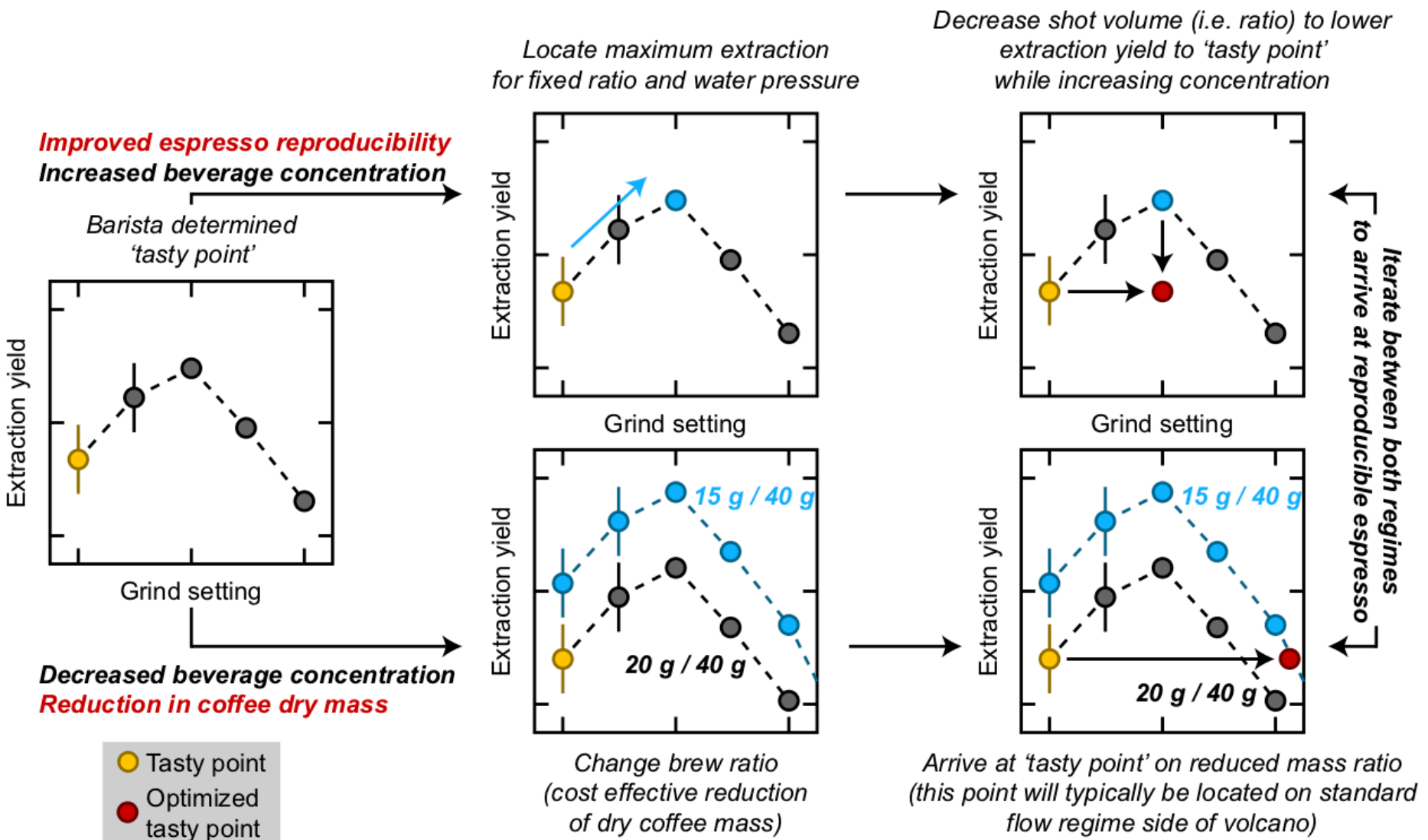


Systematic reduction of coffee mass



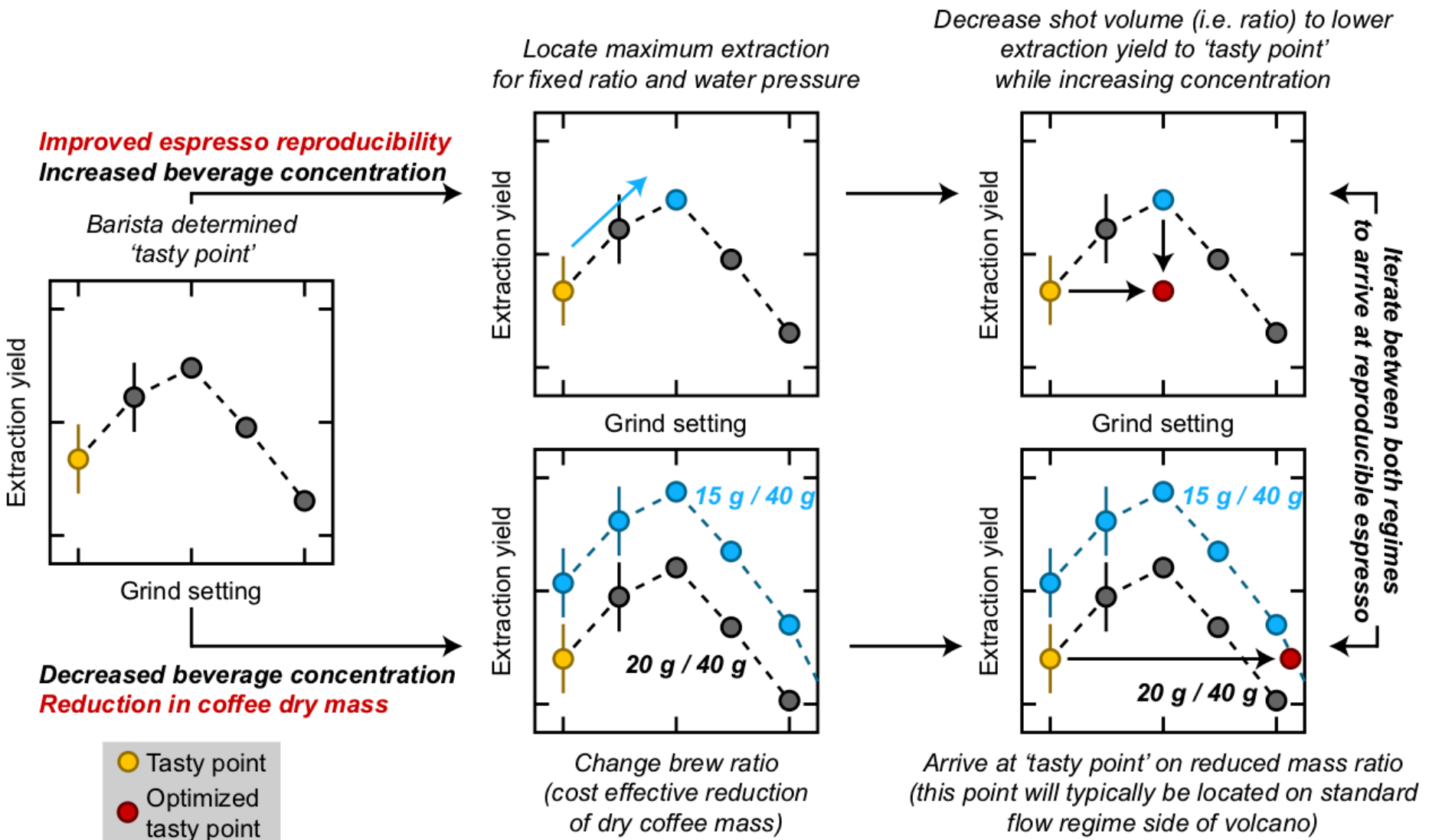


Iterative reduction of coffee waste and improved espresso





Reducing coffee mass changes concentration / mouth feel





Implications, Conclusions, and Future Directions

- Many biochemical unanswered questions in processing (Nature/Pulped/Washed), as well as fermentation stage.
- No quantitative roasting studies on flavor development
- Very few relevant studies on extraction kinetics
- Room for improvement in grinder manufacturing
- Hundreds of other exciting questions, which are the basis for both my coffee lab and also the UC Davis endeavor



The collaborators

Roasters

George Howell (Boston, MA)
Colonna (Bath, England)
Roseline (Portland, OR)
Tailored (Eugene, OR)
Supreme (Brisbane, Australia)
Spark (Sendai, Japan)
Gracenote (Boston, MA)
Counter Culture (Durham, NC)
Kittel (Montreal, Canada)
Lomi (Paris, France)
Belleville (Paris, France)
Stephen Leighton (Stafford, UK)

Baristas

Maxwell Colonna-Dashwood
Lesley Colonna-Dashwood
Michael Cameron
Dechen Morisco
Brian Sung

Benjamin Put
Charlotte Malaval
Ben Kaminsky
Kyle Ramage
Matt Lewin
Craig Simon
Jérôme Grenier-Desbiens
Hidenori Izaki
Matthew Perger

Equipment manufacturers

Beckman Coulter
Mahlkönig
San Remo
Puqpress
La Marzocco
Reg Barber

Academics

Jamie Foster (Portsmouth, UK)
William Lee (Huddersfield, UK)
Justin Wilkinson (Cambridge, UK)
Zachary C. Kennedy (PNNL, WA)
Sean A. Fontenot (Oregon, OR)
Brent Melot (USC, CA)
Keith, T. Butler (Oxford, UK)
Rory W. Speirs (Melbourne, AUS)

And many many more



Some actionable information

Brew recipe: **60 g of coffee / L**

The most common mistake in home brewing is using too little coffee and extracting for too long

Coarse grind (French Press, 4 min)

Medium grind (pour over, 2.5 min)

fine grind (Aeropress, 1.25 min)

Water chemistry: **Start with RO/DI/Milli-Q water**

Keep bicarbonate below 50 mg/L

0.25 g/L $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ (epsom salt)

~25 ppm Mg^{2+} as Mg^{2+}

0.05 g/L NaHCO_3 (baking soda)

~35 ppm HCO_3^- as HCO_3^-

Coffee preference: *VERY APPROXIMATELY*

Acidic = East Africa, Chocolate and nuts = South/Central America