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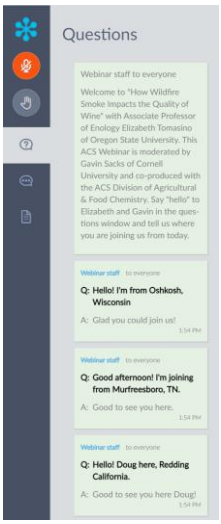

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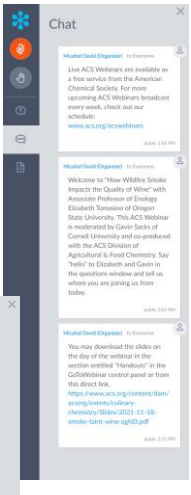

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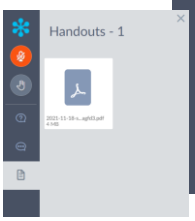

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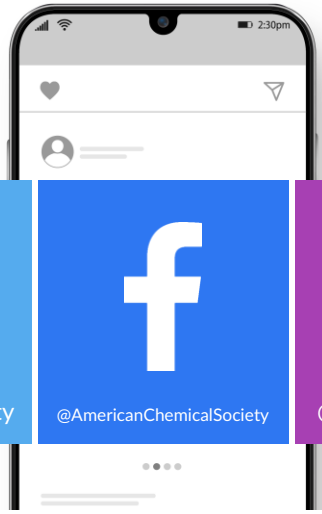

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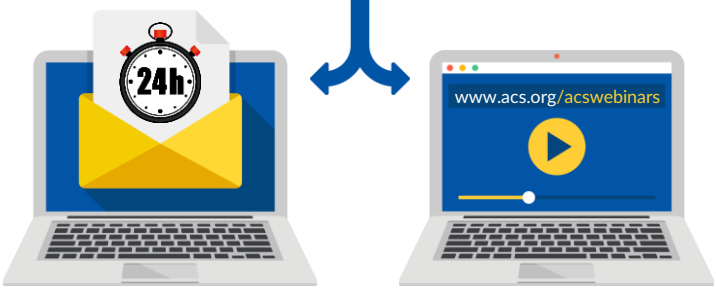

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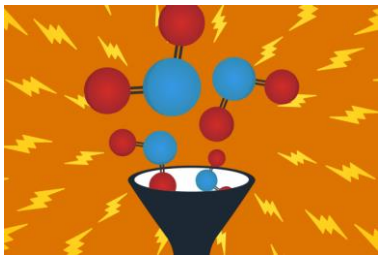

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Sam Jones, PhD
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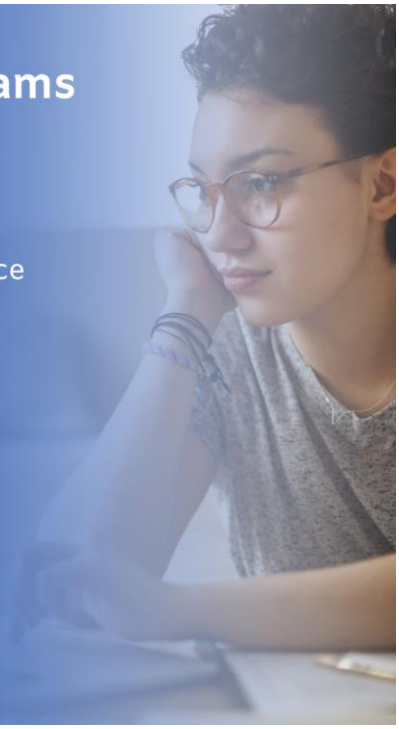

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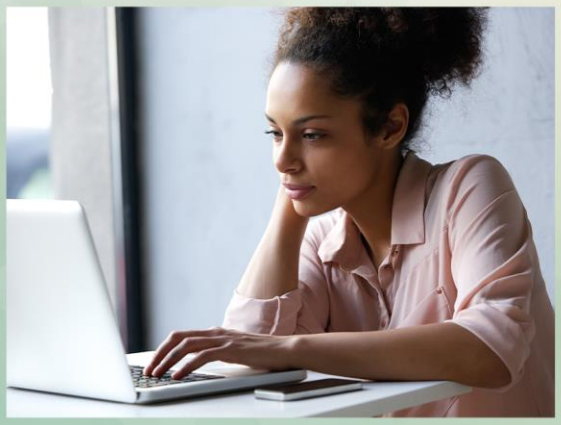

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9

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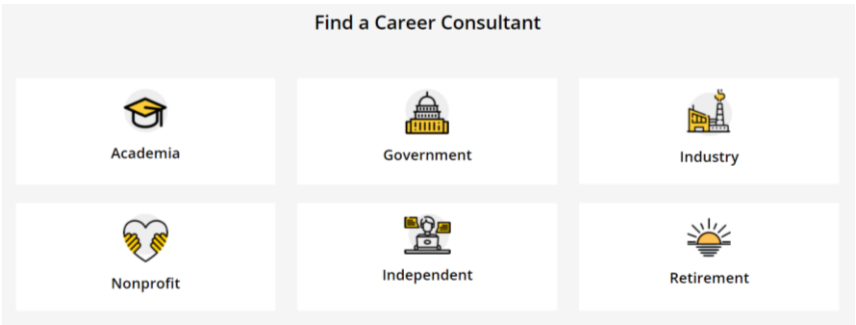

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11

12

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ACS Scholar Adunoluwa Obisesan

BS, Massachusetts Institute of Technology, June 2021
(Chemical-biological Engineering, Computer Science & Molecular Biology)

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15

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Chocolate Chemistry

MATT HARTINGS

Associate Professor, Chemistry, American University and Author, "Chemistry in Your Kitchen"

CORDELIA RUNNING

Assistant Professor, Nutrition & Food Science, Purdue University

TOM CONNELLY

Executive Director and CEO, ACS

ROBERT YOKLEY

Chair, Senior Chemists Committee, ACS

ARLENE GARRISON

Past Chair, Senior Chemists Committee, ACS

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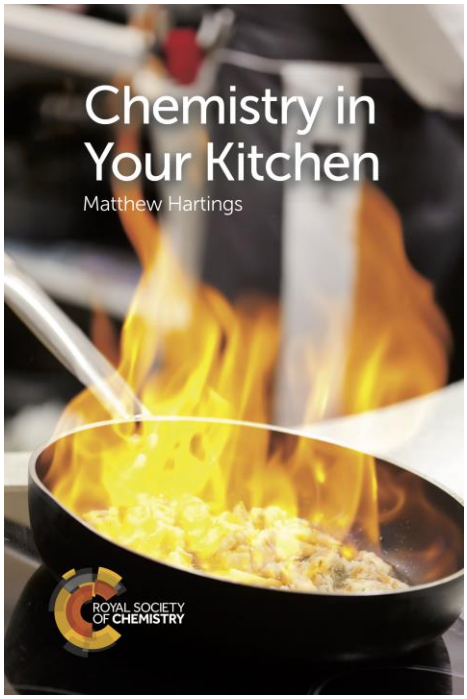
16



Temperamental Chocolate

AMERICAN

17

Things to remember: Cocoa Powder

Cocoa Powder is > 50% carbohydrates (starches and fibers)

It will absorb water (can't just add cocoa to a recipe without adjusting liquid)

Liquid with cocoa powder will thicken/expand
Gelatinization Temperature 61-68 ℃

Schmieder and Keeney
Journal of Food Science **1980**

Image Credit: Vicky Wasik – Serious Eats

Dutch Process (Alkalized) Cocoa Powder

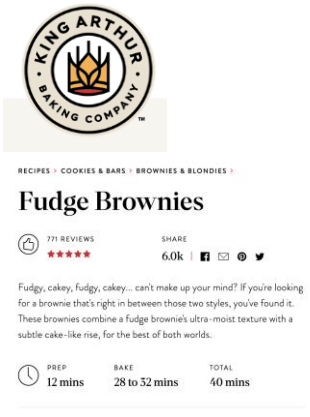
More intense/deeper flavor

Mind your leavening agents and added acids

18

Fun Recipes

https://www.seriouseats.com/eggless-chocolate-mousse

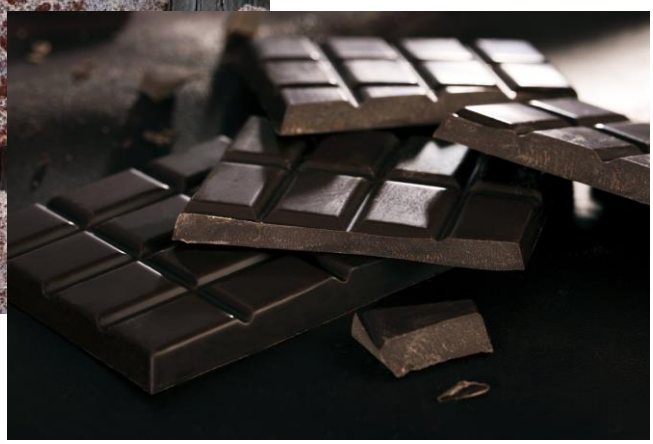


https://www.kingarthurbaking.com/recipes/fudge-brownies-recipe

19

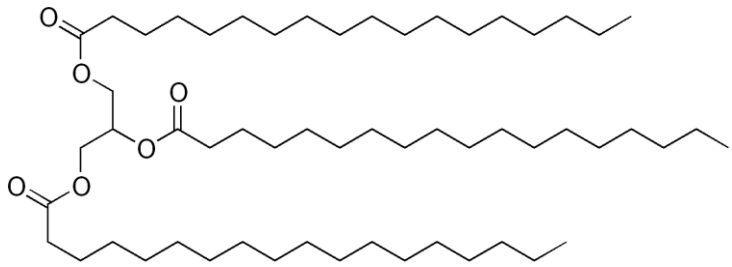
Image Source: Gilco Ingredients

Image Source: Cocoa Loco



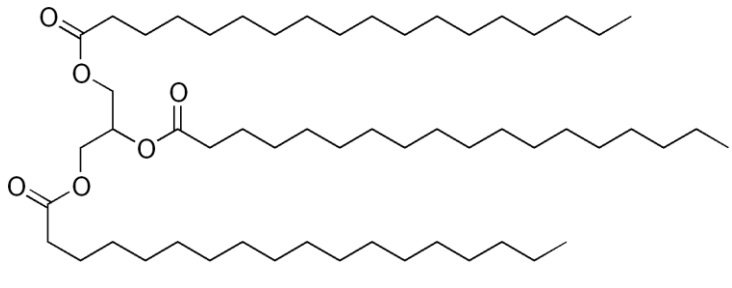
20

Tristearin



21

Tristearin



Palmitic
C_{16}

Stearic
C_{18}

Oleic
C_{18}

22

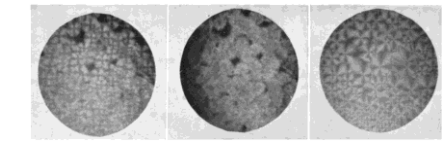
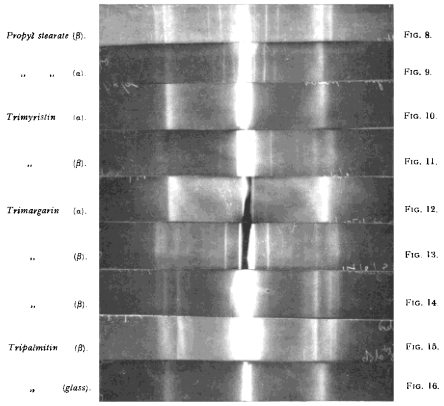
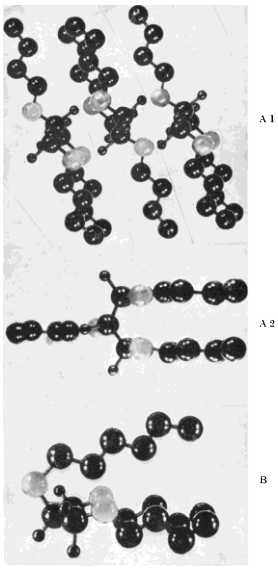


FIG. 5. *Trilaurin α.* FIG. 6. *Trilaurin β.* FIG. 7 *Tristearin α.*





Clarkson and Malkin
***Journal of the Chemical Society* 1934**

23

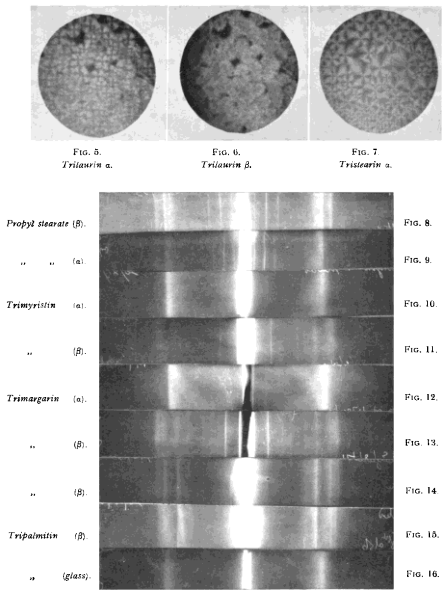
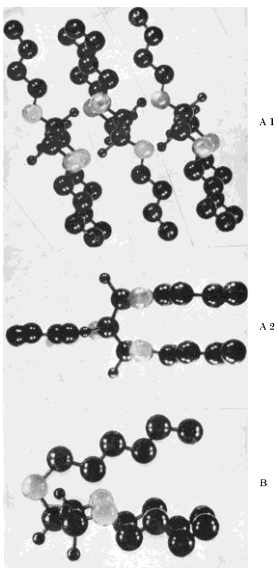
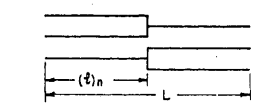


FIG. 5. *Trilaurin α.* FIG. 6. *Trilaurin β.* FIG. 7 *Tristearin α.*

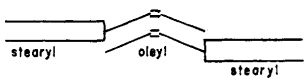


Clarkson and Malkin
***J Chem Soc* 1934**

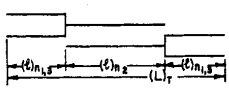
structures, one for a fatty acid and another for mixed triglyceride.



(a) Simple triglyceride



(a) 2-Oleyldistearin

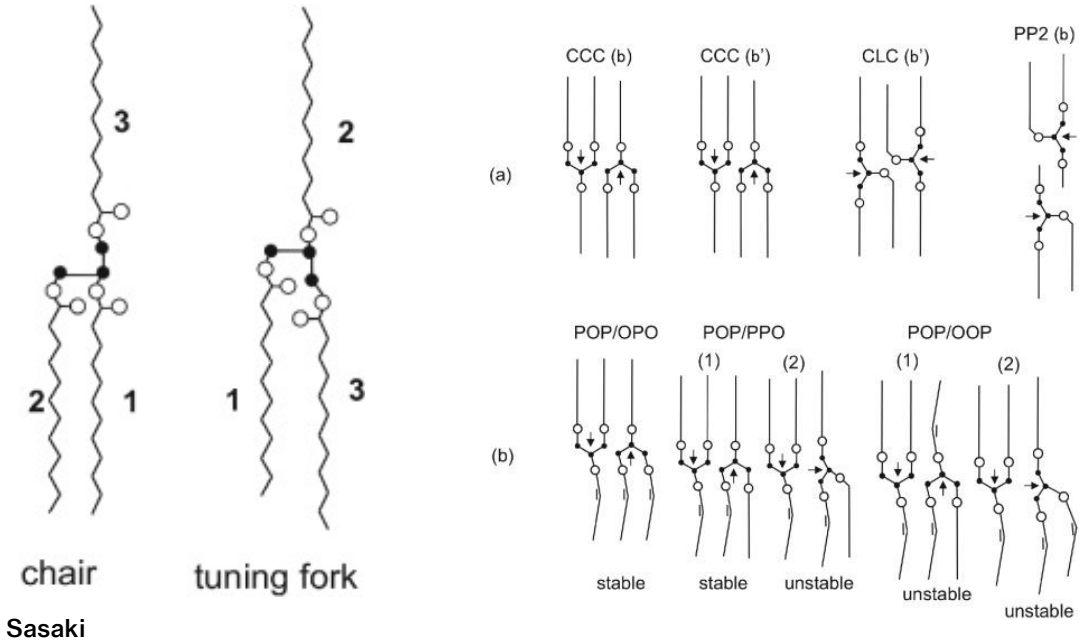


(b) Symmetrical or "tuning fork" arrangement

(c) Unsymmetri-

Lutton
***J Am Chem Soc* 1948**

24



Sasaki
***Cocoa Butter and Related Compounds* 2012**

25

f Dark Chocolate

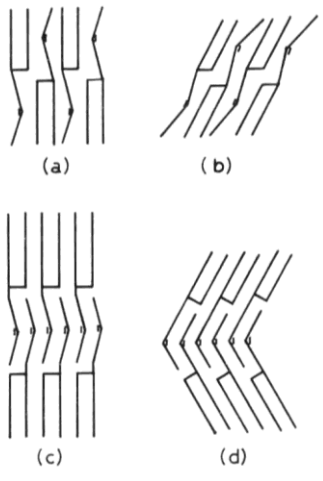


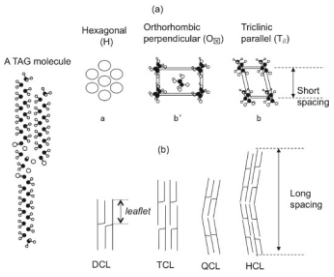
Figure 2. Postulated structure models of POP poly-

Image Source: Gilco Ingredients

Koyano
***Food Structure* 1990**

26

		Melting Point (°C)	Subcell Structure	Structure Chain Length
γ	I	17.3		double
α	II	23.3	H	double
β□	III	25.5	$O_{\perp}$	double
β□	IV	27.5	$O_{\perp}$	double
β	V	33.8	$T_{\parallel}$	triple
β	VI	36.3	$T_{\parallel}$	triple



Sasaki
Cocoa Butter and Related Compounds **2012**

27

As early as **1500 BCE** - Olmec Civilization
Chocolate agriculture/use

1519 CE - Hernán Cortés

1828 CE - Coenrad Johannes van Houten
Chocolate Press

1847 CE - Joseph Fry
First chocolate bar

Aztec woman pouring chocolate
Codex Tudela **16th Century**

Champurrado (Chocolate Atole)
Recipe via María del Mar Cuadra

1/3 cup masa harina
2 cups warm water
2 cups milk
3 oz finely chopped chocolate
3 oz piloncillo
dash salt
2 star anise pods
2 cinnamon sticks

Whisk masa harina and water until combined in a pot over medium heat. Stir in milk, chocolate, piloncillo, and salt. Add anise and cinnamon. Bring to a simmer. Cook, stirring occasionally until chocolate is melted and thickened. Discard anise and cinnamon. Serve.

28

		Melting Point (°C)	Subcell Structure	Structure Chain Length
γ	I	17.3		double
α	II	23.3	H	double
β'	III	25.5	$O_{\perp}$	double
β'	IV	27.5	$O_{\perp}$	double
β	V	33.8	$T_{\parallel}$	triple
β	VI	36.3	$T_{\parallel}$	triple

Finely chop chocolate

Place 2/3 in a double boiler → **Heat to over 40 °C** → **Remove from heat and add final 1/3** → **Cool to 28 °C with stirring** → **Heat to 32 °C with stirring** → **Remove from heat test for temper.**
Some chocolate spread on wax paper should be uniform

29

https://www.seriouseats.com/the-food-lab-best-way-to-temper-chocolate

30

Chocolate, Chemosensation, and Saliva

Cordelia Running, PhD
Purdue University

Acknowledgements & Funding

Students:


Ciera Crawford, MS


Li-Chu Huang, MS


Lissa Davis, PhD candidate

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Running USDA Hatch No 1013624, Hayes PEN04565
NIH NIDCD Early Career R21DC017559

Disclosures

Occasional consulting for food and salivary analysis companies. None connected to these projects.

32

Chocolate has a useful mix of constituents.

Darker, "healthier" chocolate has more bitter polyphenols and fiber.

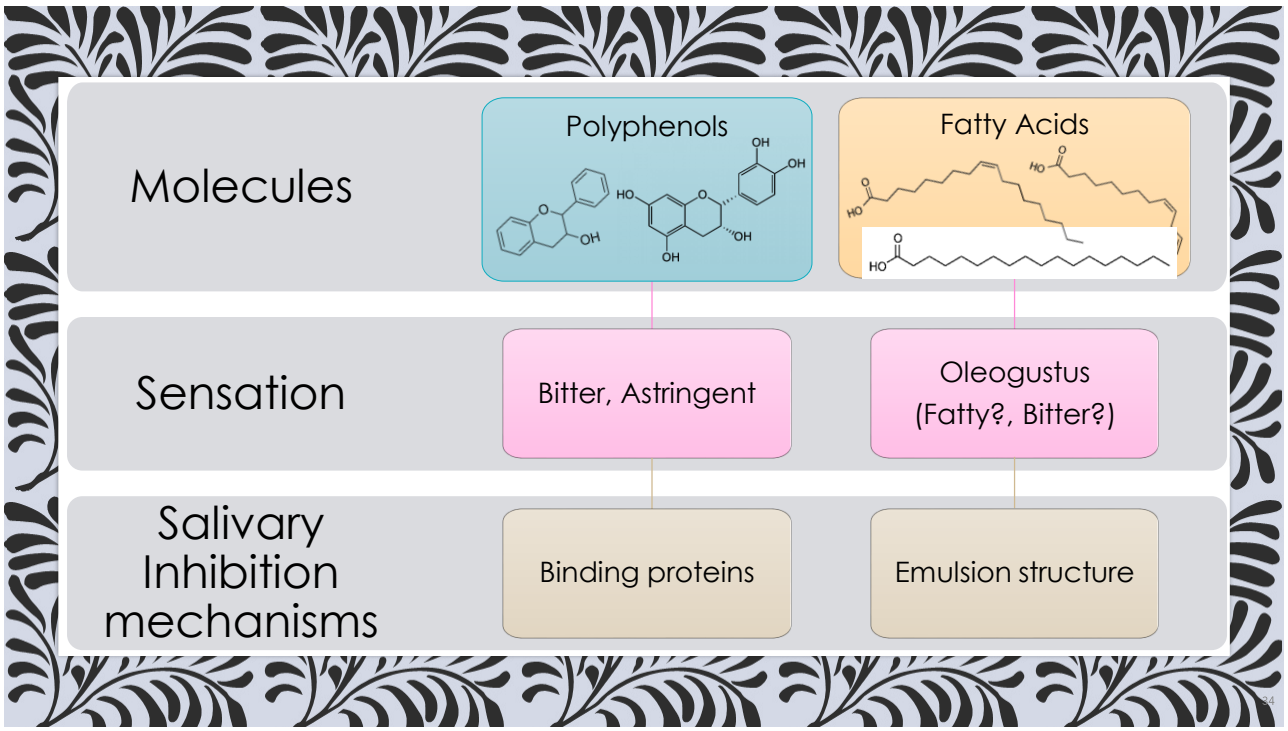
Also, less sugar and more fat.

Images from https://www.ghirardelli.com/

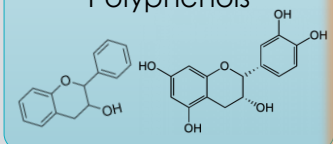
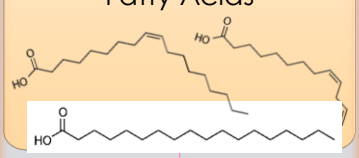
	Milk, <40%	Dark, 60%	Darker, 72%
Polyphenols* (per 32 g serving)	<1.3 mmol*	~1.8 mmol*	~2.2 mmol*
Fiber (per 32 g serving)	<1 g	3 g	3 g
Sugar (per 32 g serving)	18 g	12 g	8 g
Fat (per 32 g serving)	10 g	12 g	15 g

*Catechin equivalents estimated from: Vinson & Motisi, 2015 https://doi.org/10.1016/j.jff.2014.12.022

33



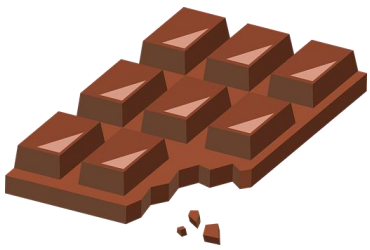
34

Molecules	Polyphenols 	Fatty Acids 
Sensation	Bitter, Astringent	Oleogustus (Fatty?, Bitter?)
Salivary Inhibition mechanisms	Binding proteins	Emulsion structure

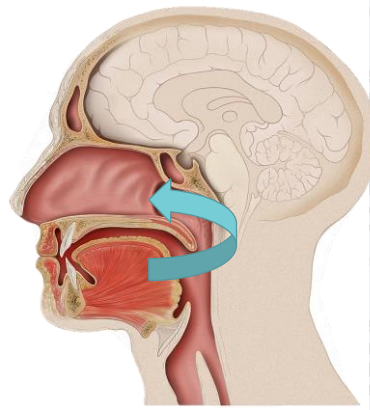
Oleogustus – Actual taste from fatty acids

- Taste ≠ Flavor
- Much of flavor is actually retronasal olfaction

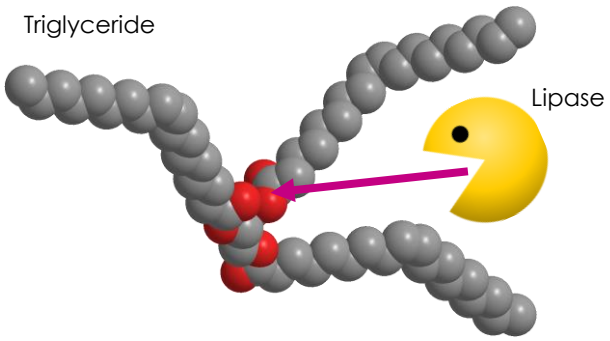
Flavor:
Chocolate!



Taste:
Sweet
Bitter
Fatty?

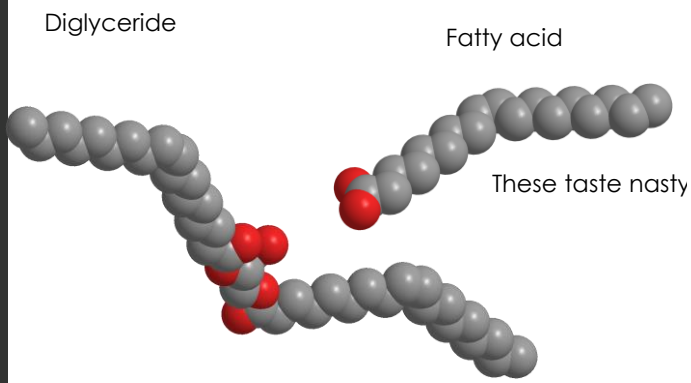


Oleogustus is the taste sensation stimulated by free fatty acids.



37

Oleogustus is the taste sensation stimulated by free fatty acids.



From Running, Craig, and Mattes 2015; extra data

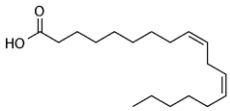
38

Used chocolate substitute (melting wafers) to study relationship with how saliva creates emulsions, and how that relates to taste intensity

(2020 study, during fall of COVID19 pandemic year 1)

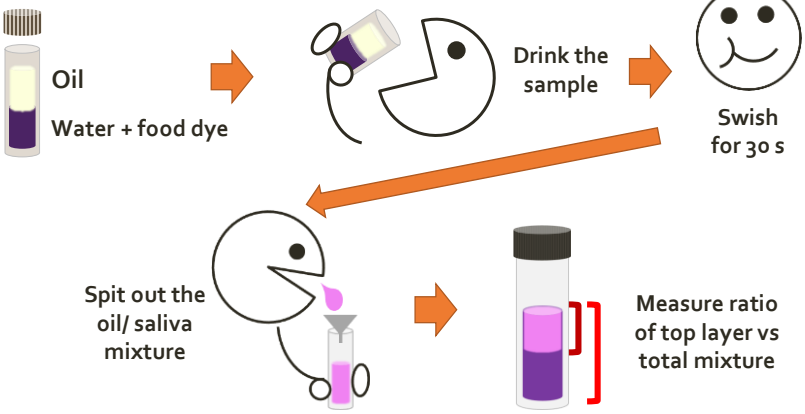
Li-Chu Huang, MS

+ linoleic acid



←Can people tell them apart?

← How strong is the taste?



39

Examples of spat out samples from two different individuals—at the same time point!

Li-Chu Huang, MS

40

Hypothesis

Finer salivary emulsions correlate with better ability to detect fatty acids, and more intense sensation.

41

Fat layer size associated with several sensory and dietary patterns.

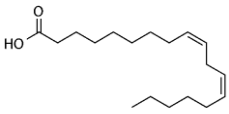
Li-Chu Huang, MS

More stable emulsion associated with

greater taste intensity rating of linoleic acid candies

Discriminators had larger layer sizes at 0, 0.5 min

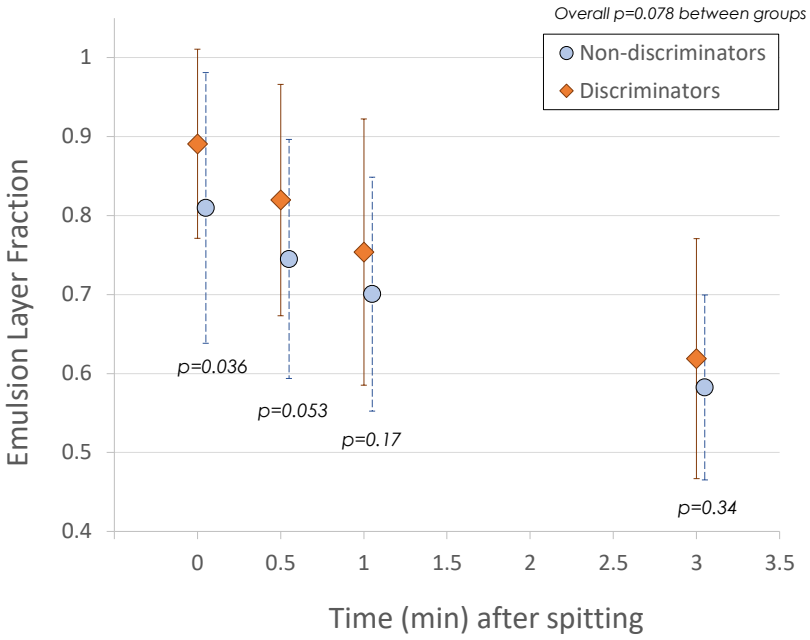
+ linoleic acid



42

People who could tell the linoleic acid spiked candy apart from the plain candy had larger upper layers early after spitting.

Implies their saliva makes better emulsion.



43

Hypothesis

Finer salivary emulsions correlate with better ability to detect fatty acids, and more intense sensation.

44

So, saliva:

- Can alter the packaging of fat in ways that influence sensory intensity and discriminatory ability for oleogustus.
- This could potentially influence other taste sensations as well, as the packaging of lipophilic vs. hydrophilic molecules would be different among people.

45

THANK YOU!

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46

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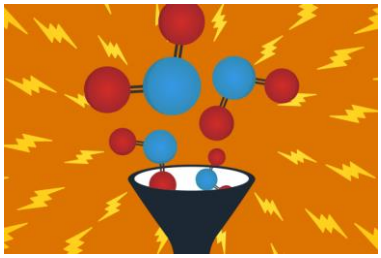

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49