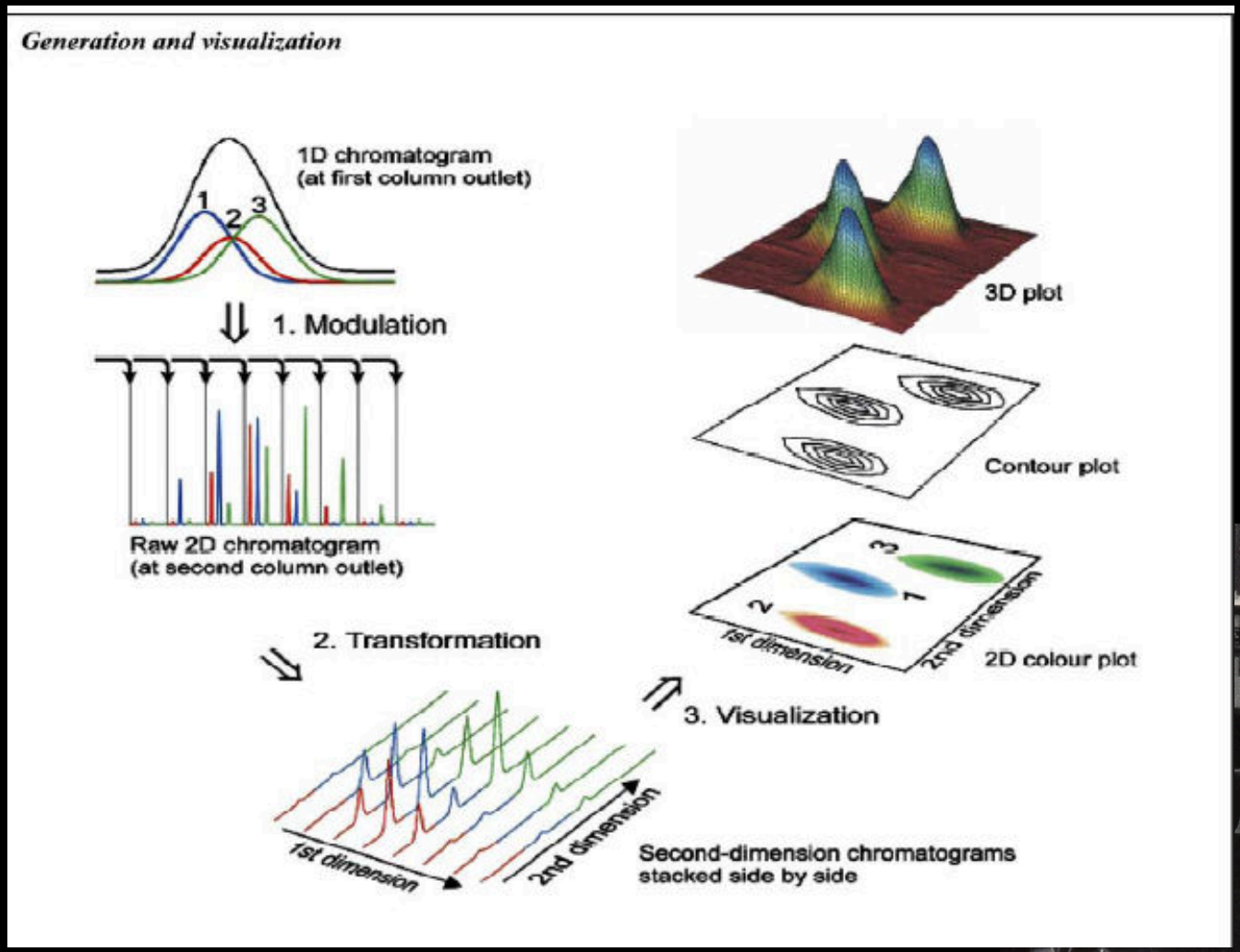
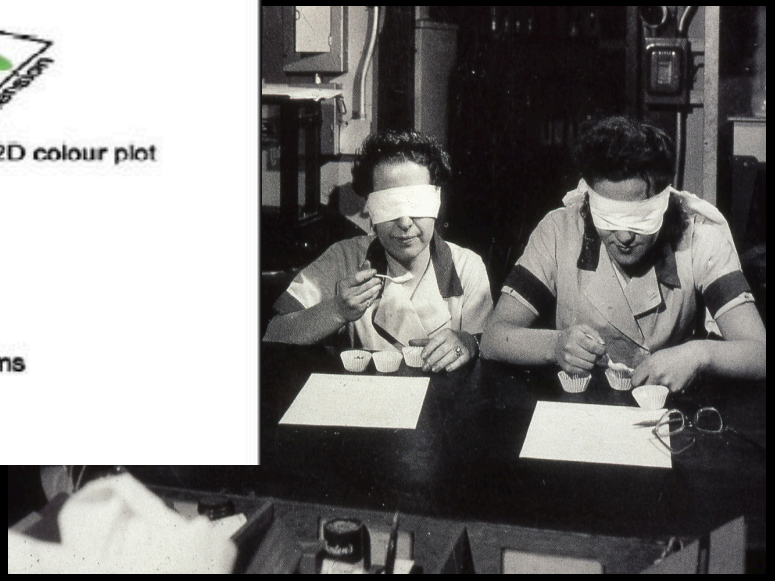
Predicting flavor perception from mixture composition

Terry E. Acree

Analytical -> Sensory



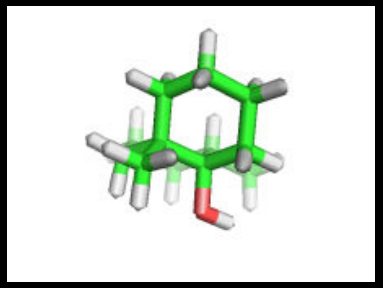
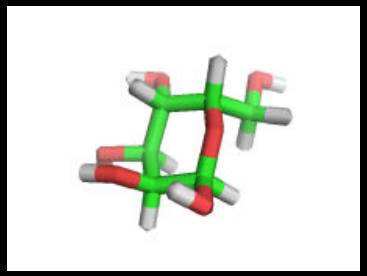


Chemosensory Perception

Flavor = f(Taste, Odor, Chemesthesis,Time)

Food odor is experienced in the mouth.
Environments are experienced in the nose.

Flavor chemicals

Sense	smell	taste	chemesthesis
Percept	earthy	sweet	astringent
Structure			
Name	geosmin	glucose	QMR
Size	< 300 Daltons	< 1000 Daltons	

The Psychophysical Model

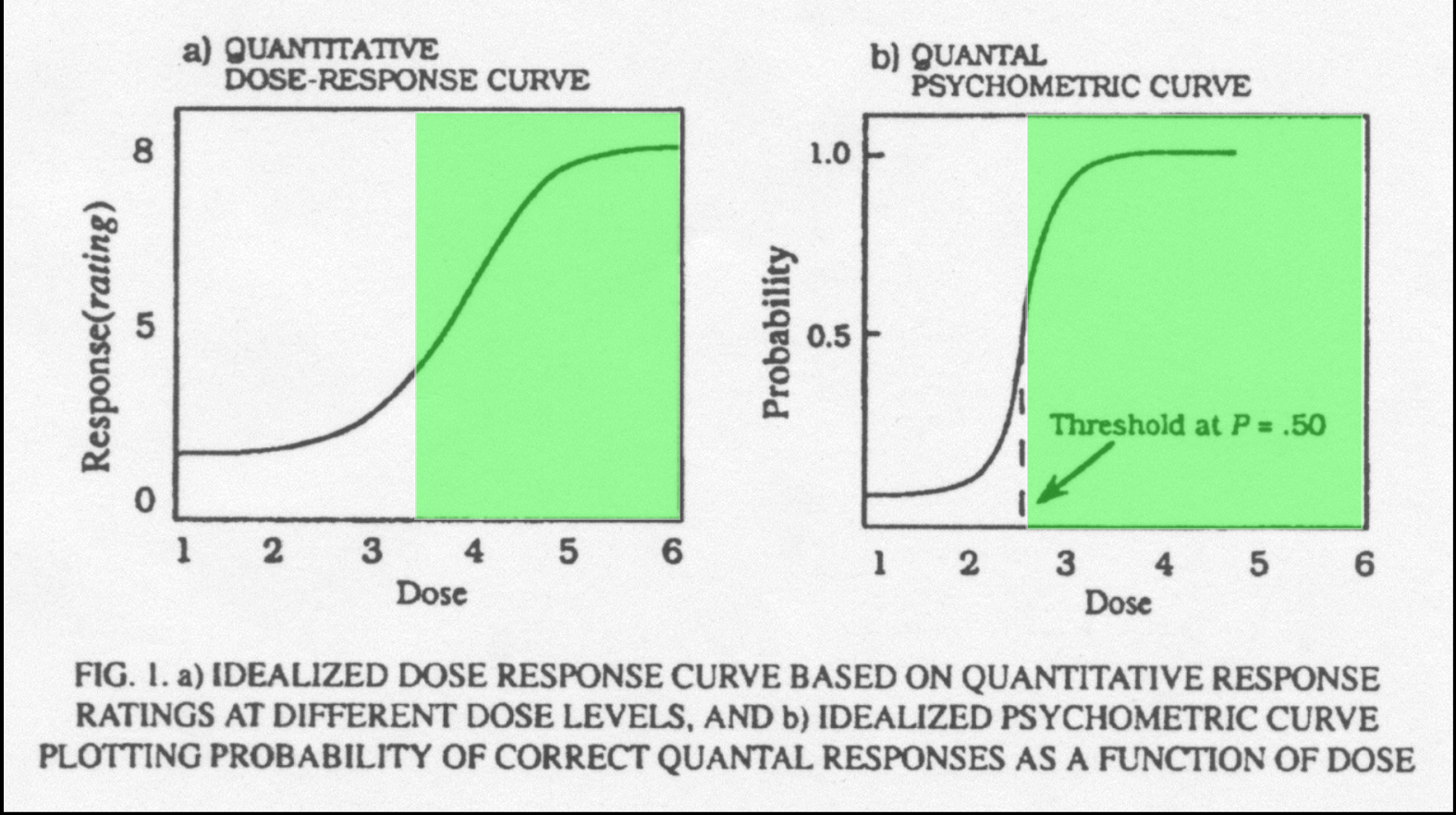
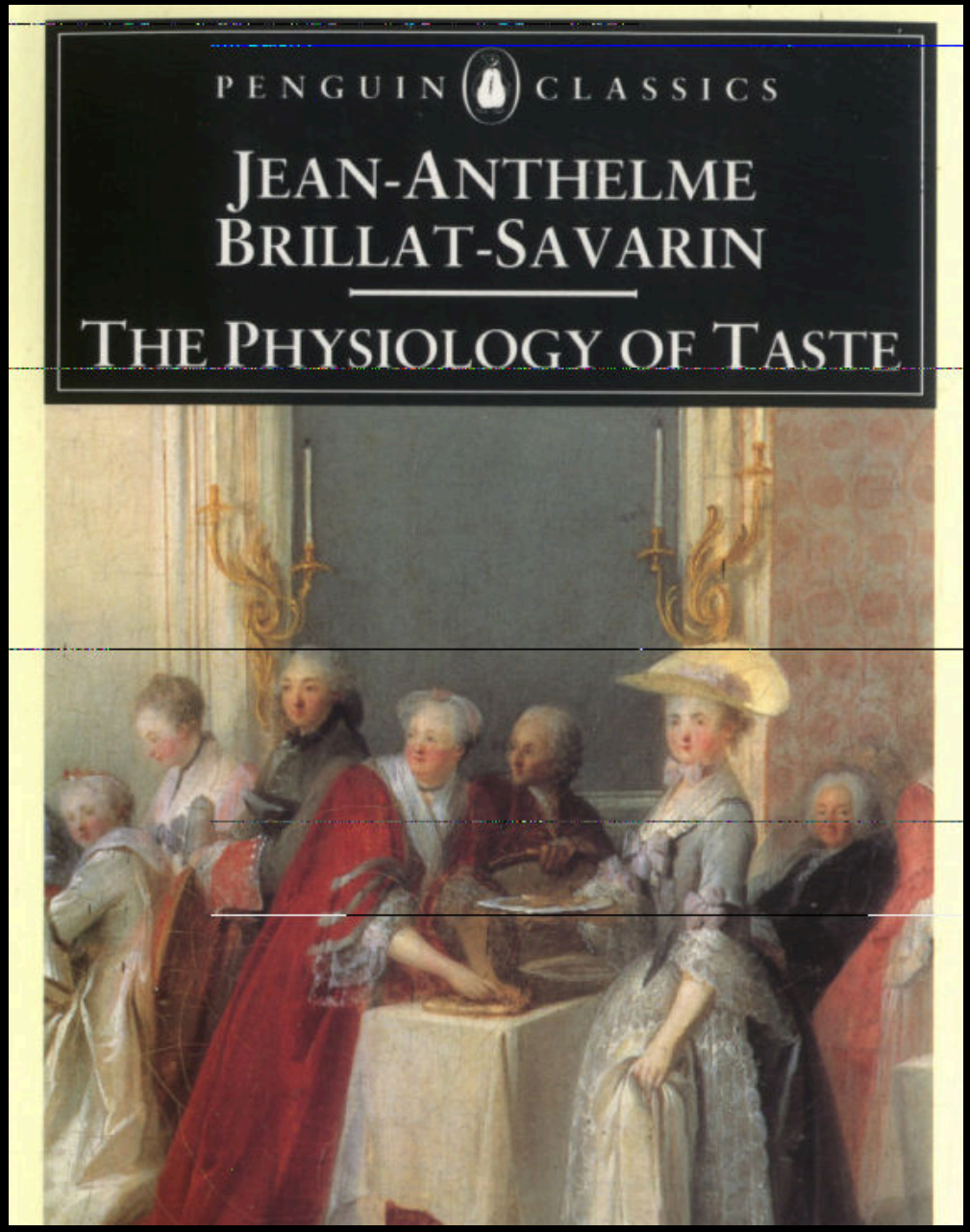


FIG. 1. a) IDEALIZED DOSE RESPONSE CURVE BASED ON QUANTITATIVE RESPONSE RATINGS AT DIFFERENT DOSE LEVELS, AND b) IDEALIZED PSYCHOMETRIC CURVE PLOTTING PROBABILITY OF CORRECT QUANTAL RESPONSES AS A FUNCTION OF DOSE

Quale = “green”

“It cannot be disputed that it is chemistry which will reveal the cause of the basic elements of [flavor] taste.” 1825



High Resolution Olfactometer - 1976

Sniffer to Determine the Odor of Gas Chromatographic Effluents

T. E. Acree,* R. M. Butts, R. R. Nelson, and C. Y. Lee

Department of Food Science and Technology, Cornell University, New York State Agricultural Experiment Station, Geneva, N.Y. 14456

Sniffing the effluent of a gas chromatograph (GC) is the most useful means of determining which components of a complex mixture of volatiles have odor. Although such a

Figure 1 shows a diagram of a sniffer constructed from a brass laboratory filter pump (A). The air supply is deodorized by an in-line charcoal (Pittsburgh activated, 12–40 mesh) filter (H) and humidified by passing the air over the surface of distilled water in a half filled

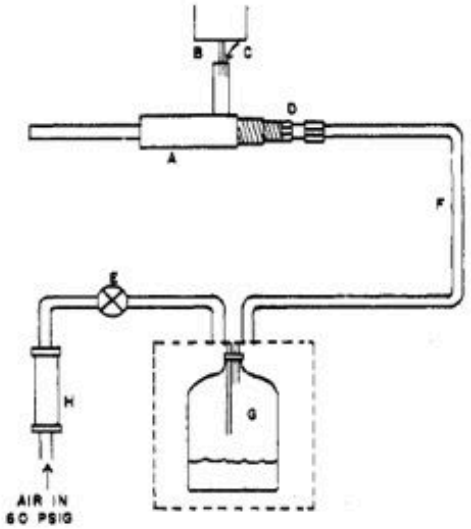
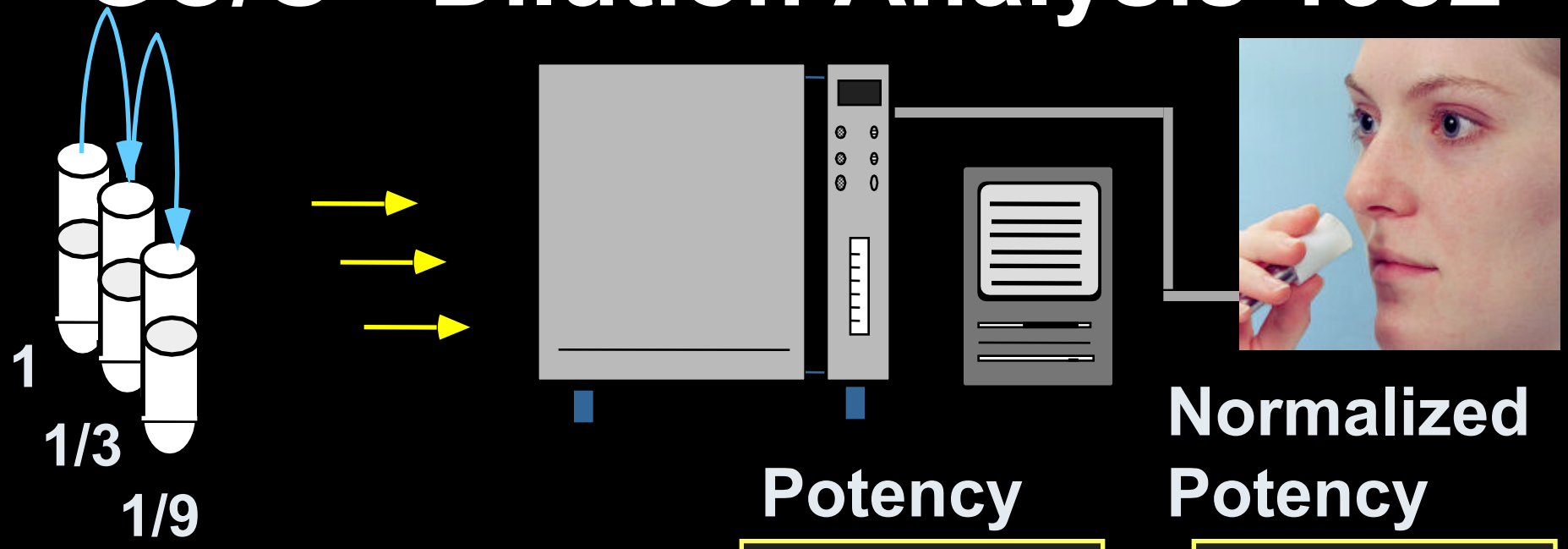
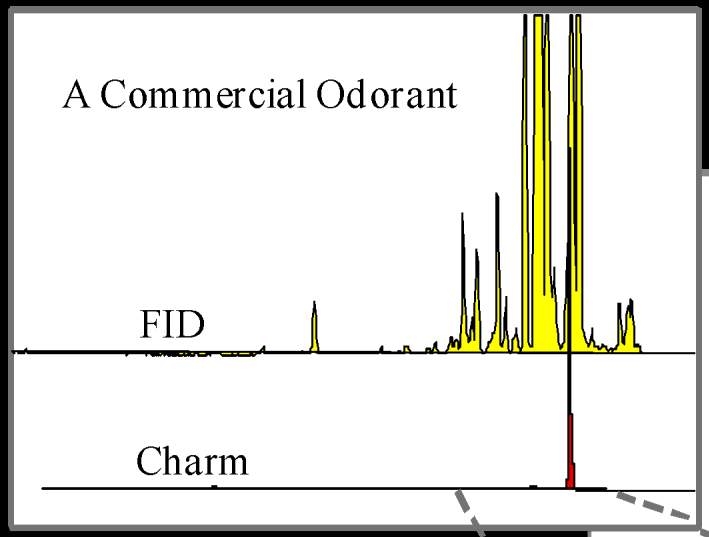


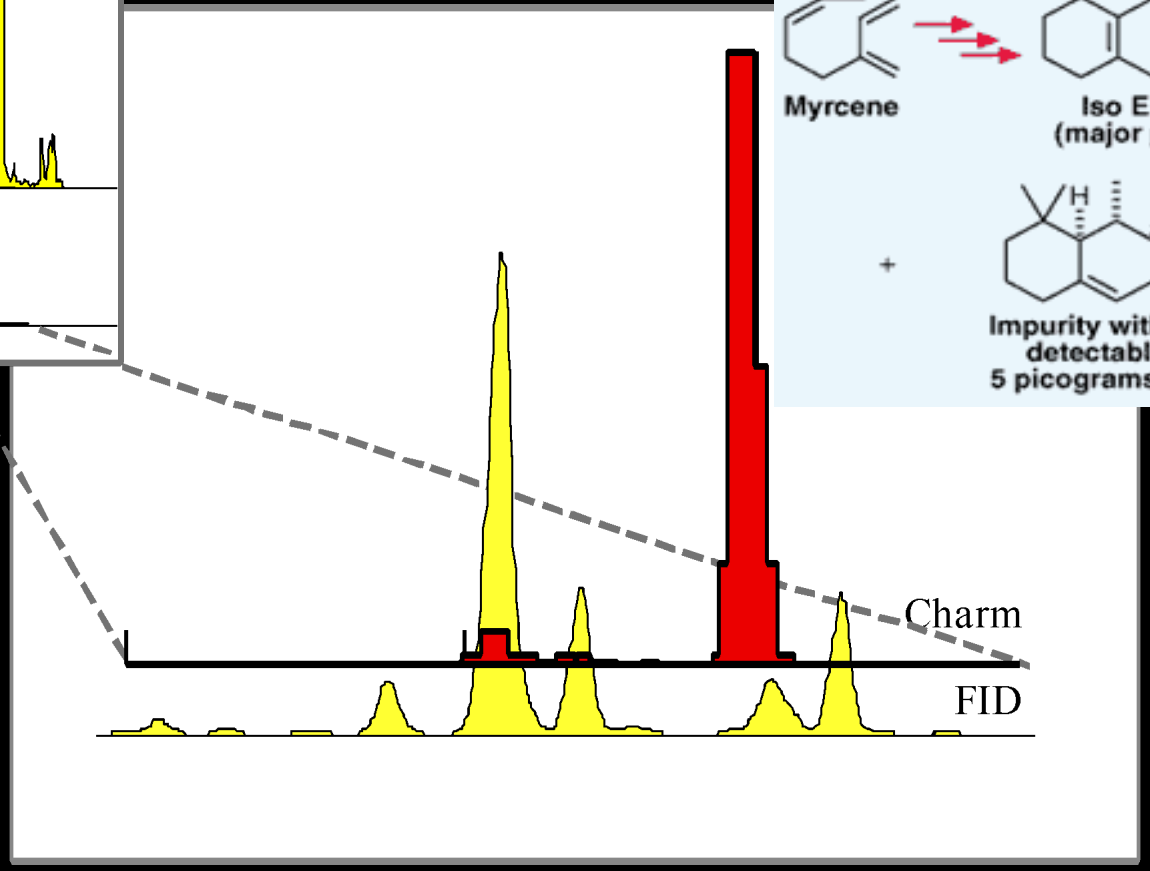
Figure 1. Diagram of the sniffer constructed from a laboratory filter pump

GC/O - Dilution Analysis 1982

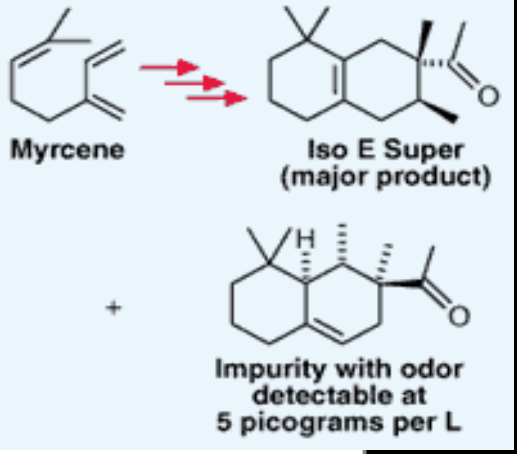


Chemical Activity vs Odor Activity
FID vs. Charm





Odorwise, impurity beats main product*



*Rouhi'00

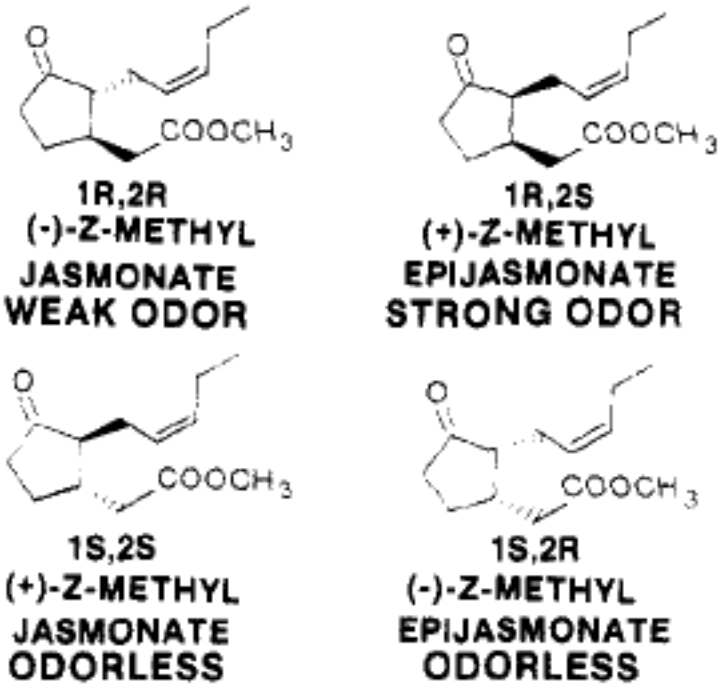


Figure 1. The four steroisomers of methyl jasmonate are shown along with odor intensity of the neat samples measured immediately after preparation.

Flavornet

http://www.flavornet.org/flavornet.htr

Address Book ▾ Bonjour ▾ Essential oils Gate Blackboard MM ▾

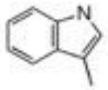
Flavornet Home | Kovats RI

CAS No	Mol Wt	Odorant
57-06-7	99	allyl isothiocyanate, allyspol, 3-isothiocya
60-12-8	122	2-phenylethyl alcohol, 2-phenylethanol,
64-17-5	46	ethanol
64-19-7	60	acetic acid
65-85-0	122	benzoic acid
66-25-1	100	hexanal
67-47-0	126	5-oxymethylfurfurole, 5-(hydroxymethyl)-
67-68-5	78	syntexan, sulfinylbis-methane, dimethyl s
67-71-0	90	dimethyl sulfone, sulfonylbismethane
71-23-8	60	propanol, 1-propanol
71-36-3	74	butanol, 1-butanol
71-41-0	88	pentanol, 1-pentanol
74-93-1	48	methanethiol, methyl mercaptan
75-07-0	44	ethanal, acetaldehyde
75-18-3	62	dimethyl sulfide
75-50-3	59	trimethylamine, N,N-dimethyl-methanami
76-22-2	152	camphor, bornan-2-one, 1,7,7-trimethylbi
76-50-6	238	bornyl isovalerate, 1,7,7-trimethylbicyclo[
78-36-4	224	linalyl butyrate, 3,7-dimethyl-1,6-octadier
78-70-6	154	linalool, 3,7-dimethylocta-1,6-dien-3-ol,2
78-83-1	74	isobutanol, 2-methyl-1-propanol
78-84-2	72	isobutyraldehyde, 2-methylpropanal
78-92-2	74	butanol, 2-butanol
78-93-3	72	methyl ethyl ketone, 2-butanone
79-09-4	74	propanoic acid, propionic acid
79-31-2	88	isobutyric acid, 2-methylpropanoic acid
79-77-6	192	β-ionone, 4-(2,6,6-trimethyl-1-cyclohexer
79-92-5	136	camphene, 2,2-dimethyl-3-methylene-bic
80-26-2	196	terpinyl acetate, α-terpineol acetate
80-56-8	136	α-pinene, 2,6,6-trimethylbicyclo[3.1.1]hep
83-34-1	131	skatole, 3-methyl-1H-indole
87-44-5	204	β-caryophyllene, [1R-(1R,4E,9S)]-4,11,1
87-91-2	206	diethyl tartrate, 2,3-dihydroxy-butanedioi

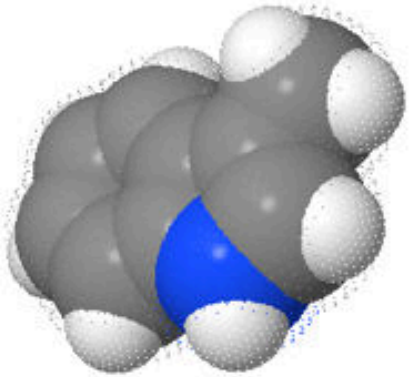
skatole 83-34-1

skatole

3-methyl-1H-indole



CAS 83-34-1 - MW 131.1



Jmol

Van der Waals surface
Fill space 80%
Spin

	OV101	DB5	OV1701	C20M
Kovats RI	[1370]	1387	1628	2484
Ethyl ester RI	[990]	988	1163	1823

[interpolated]

Percepts: mothball, fecal

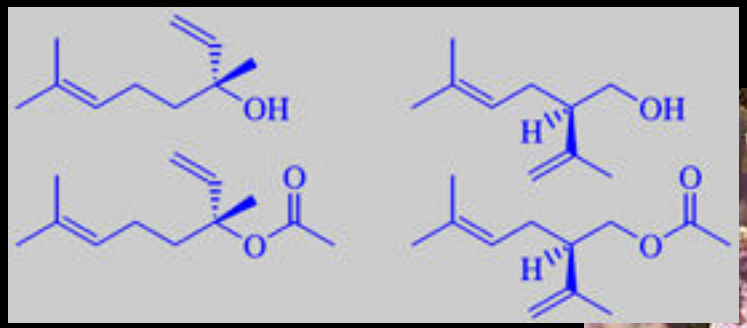
References:

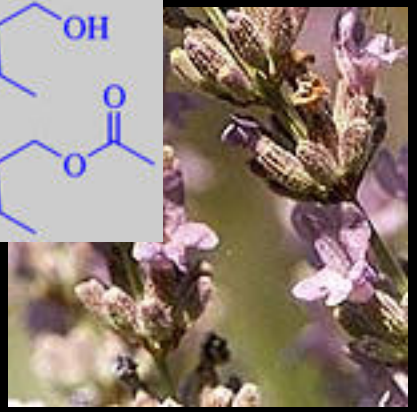
OV101

DB5 Widder, Sen & Grosch 1991; Z Lebensm Unters Forsch, 193, 32-35. Rychlik, Schieberle & Grosch Compilation of Odor Thresholds, Odor Qualities and Retention Indices of Key Food Odorants, Lichtenbergstraße, Germany, 1998. [SE-54].

Lavender

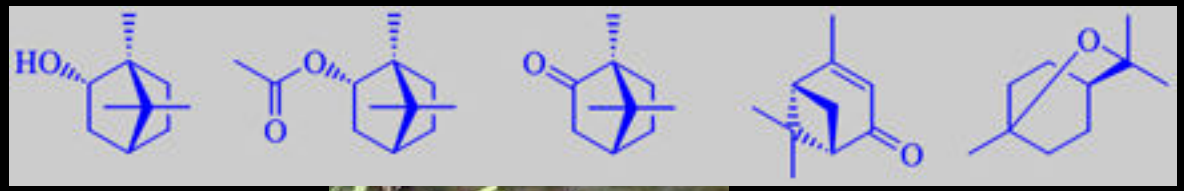
(-)-linalool,
(-)-linalyl acetate,
(-)-lavandulol
(-)-lavandulyl acetate

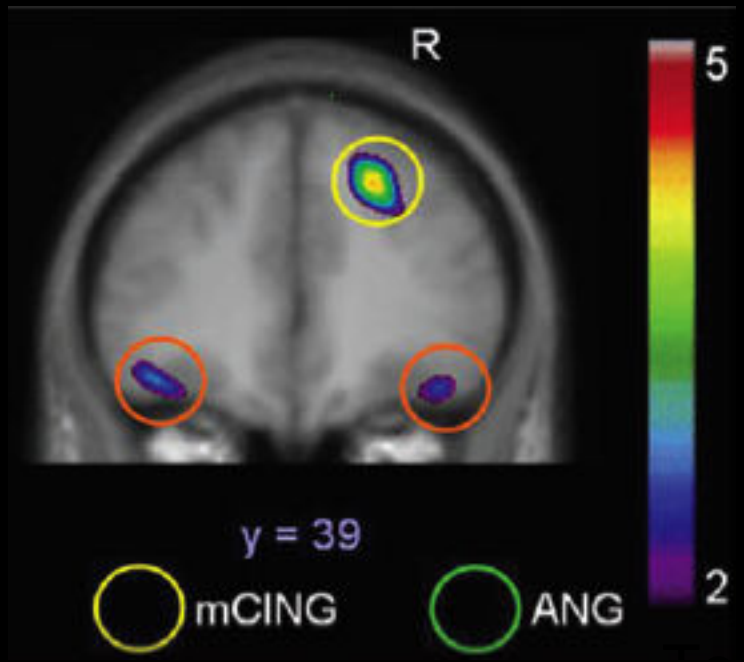


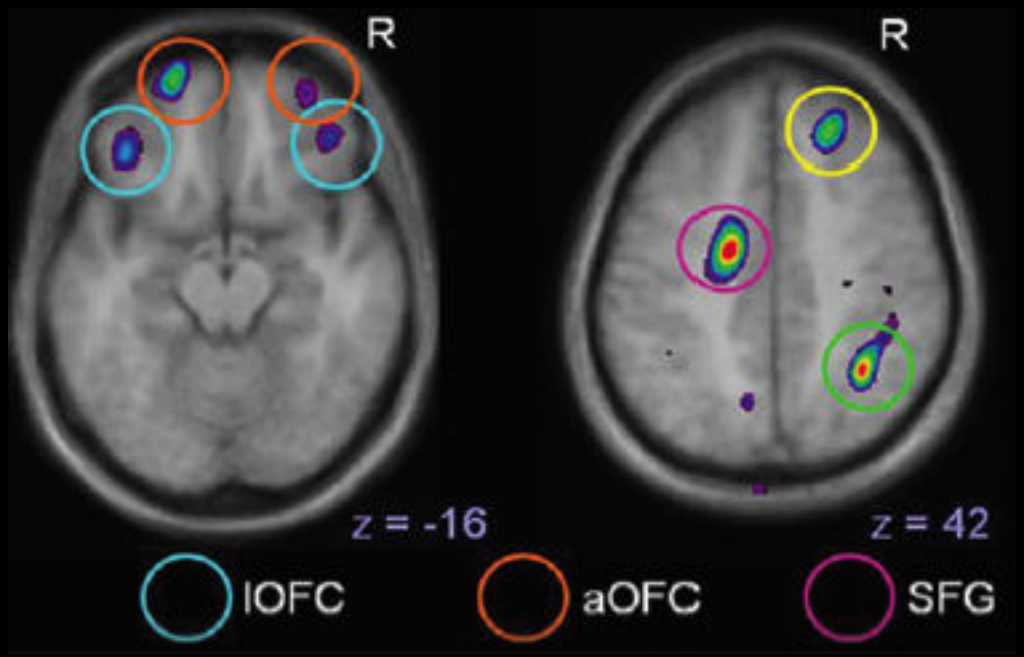


Rosemary

(+)-borneol
(+)-bornyl acetate
(+)-camphor
(-)-verbenone
1,8-cineole

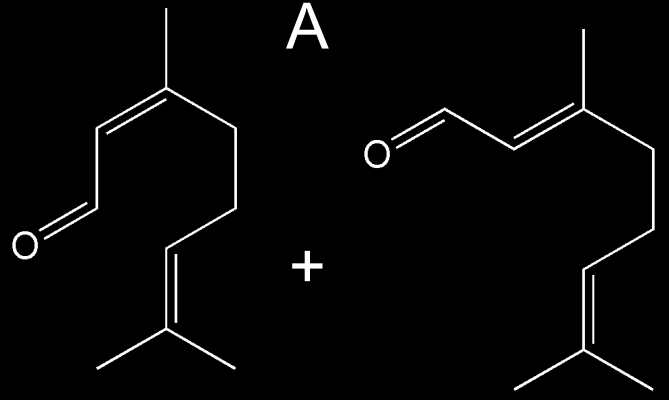






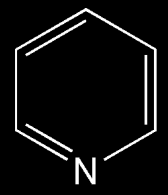
Mix - (A + B)

A



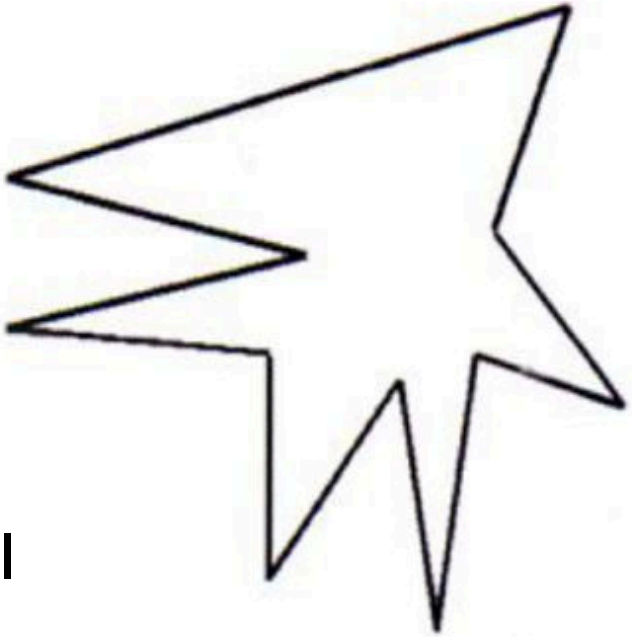
neral geranal

B



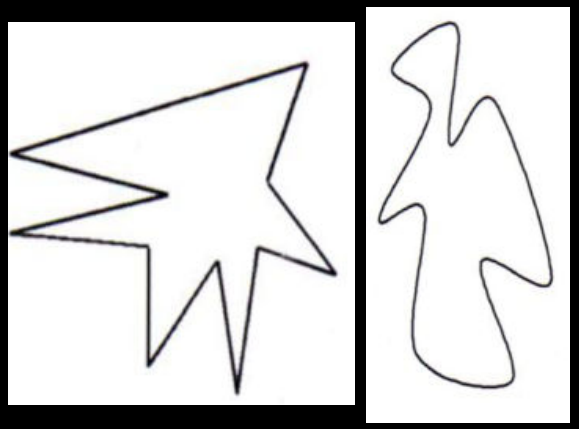
pyridine

Ramachandran 06



KiKI

BooBoo



BooBoo

KiKi

Vintage Port

Brut Champagne

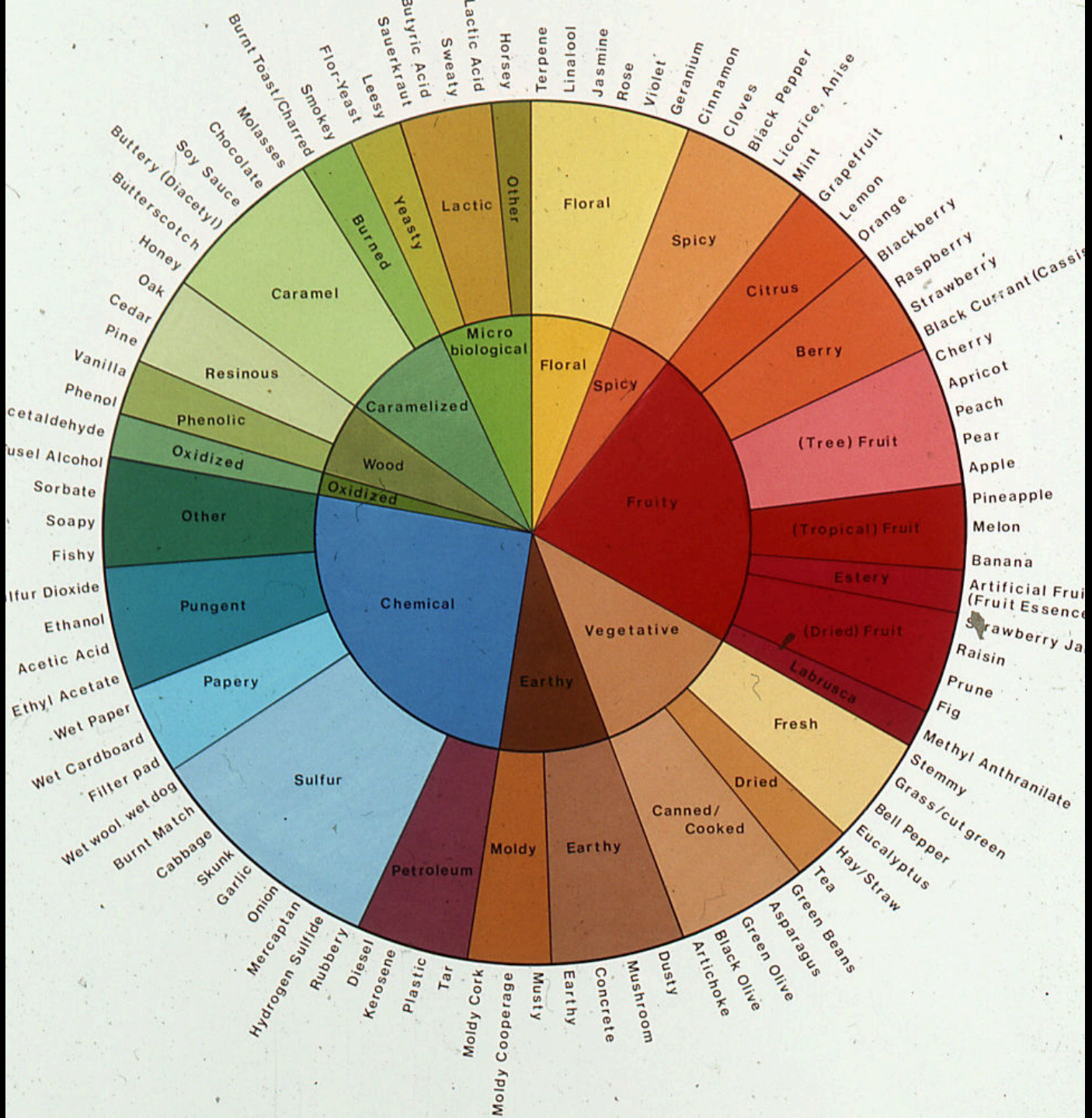
Describing flavor

Functional words

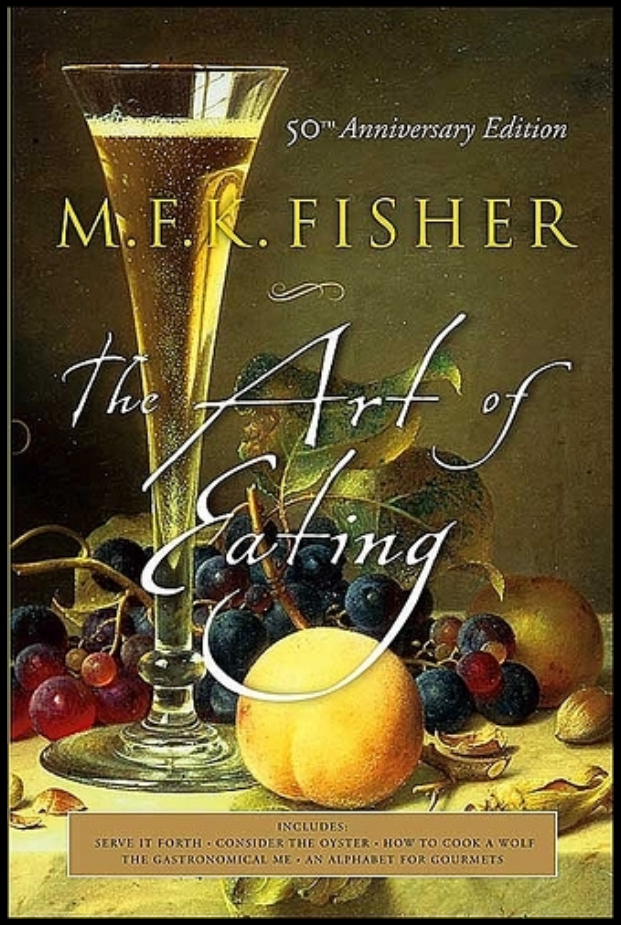
Taste
bitter, sweet, salty, sour, savory
Chemesthesis
hot , cold, astringent, burning

Associative words (~ Qualia)

Odor
pine nut, apple, melon, lobster, mushroom
...


Micro biological
Caramelized
Wood
Oxidized
Chemical
Earthy
Vegetative
Floral
Spicy
Fruity
Other
Lactic
Yeasty
Burned
Caramel
Resinous
Phenolic
Oxidized
Other
Pungent
Papery
Sulfur
Petroleum
Moldy
Earthy
Canned/ Cooked
Dried
Fresh
Labrusca
(Dried) Fruit
Estery
(Tropical) Fruit
(Tree) Fruit
Berry
Citrus
Floral
Spicy
Terpene
Linalool
Jasmine
Rose
Violet
Geranium
Cinnamon
Cloves
Black Pepper
Licorice, Anise
Mint
Grapefruit
Lemon
Orange
Blackberry
Raspberry
Strawberry
Black Currant (Cassis
Cherry
Apricot
Peach
Pear
Apple
Pineapple
Melon
Banana
Artificial Frui
(Fruit Essence
Strawberry Ja
Raisin
Prune
Fig
Methyl Anthranilate
Stemmy
Grass/cutgreen
Bell Pepper
Eucalyptus
Hay/Straw
Tea
Green Beans
Asparagus
Green Olive
Black Olive
Artichoke
Dusty
Mushroom
Concrete
Earthy
Musty
Moldy Cooperage
Moldy Cork
Tar
Plastic
Kerosene
Diesel
Rubbery
Hydrogen Sulfide
Mercaptan
Onion
Garlic
Skunk
Cabbage
Burnt Match
Wet wool, wet dog
Filter pad
Wet Cardboard
Wet Paper
Ethyl Acetate
Acetic Acid
Ethanol
lfur Dioxide
Fishy
Soapy
Sorbate
usel Alcohol
cetaldehyde
Phenol
Vanilla
Pine
Cedar
Oak
Honey
Butterscotch
Buttery (Diacetyl)
Soy Sauce
Chocolate
Molasses
Burnt Toast/Charred
Smokey
Flor-Yeast
Leesy
Sauerkraut
Butyric Acid
Sweaty
Lactic Acid
Horsey

Born 100 years ago



“ Food is not a metaphor for life. It is life, and eating is an art.”

Analysis

The smell of Dijon gingerbread.
by M. F. K. Fisher

"Its flat strange odor, honey, cow dung, clove, something unnameable but unmistakable, blew all over the town." - from "Two birds without a branch"

TABLE 2

PERCENT CORRECT JUDGEMENTS OF THE COMPONENTS IN STIMULI

No. of Odors Correctly Identified	No. of Odors Presented				
	1	2	3	4	5
0	18.2*	9.0	4.0	3.1	0.7
1	81.8†	55.7	34.0	28.1	14.7
2	0	35.2	48.0	43.3	48.3
3	0	0	14.0	22.0	31.5
4	0	0	0	3.7	4.9
5	0	0	0	0	0
n‡	154	122	100	164	143

*Row 1 shows the percent of judgements that were entirely incorrect.

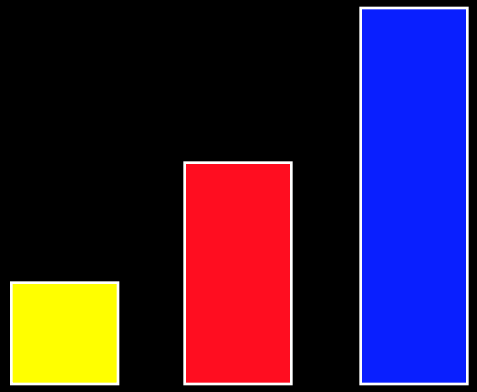
†Rows 2–6 show the percent of judgements that were correct but additional odors may also have been incorrectly selected.

‡Number of judgements when a particular number of odorants were presented, e.g., column 2 indicates there were 154 judgements of single odor stimuli.

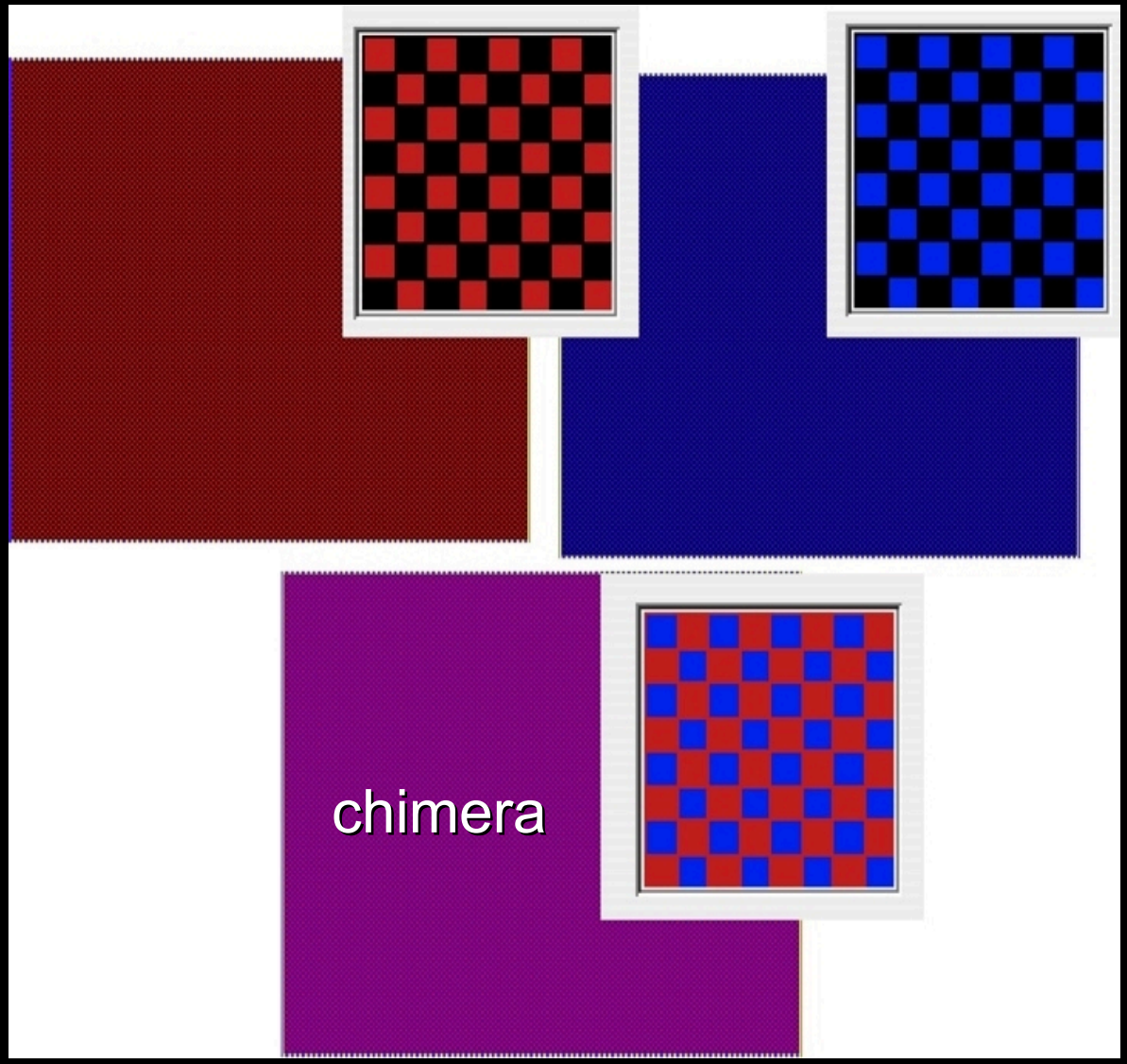
Laing 89

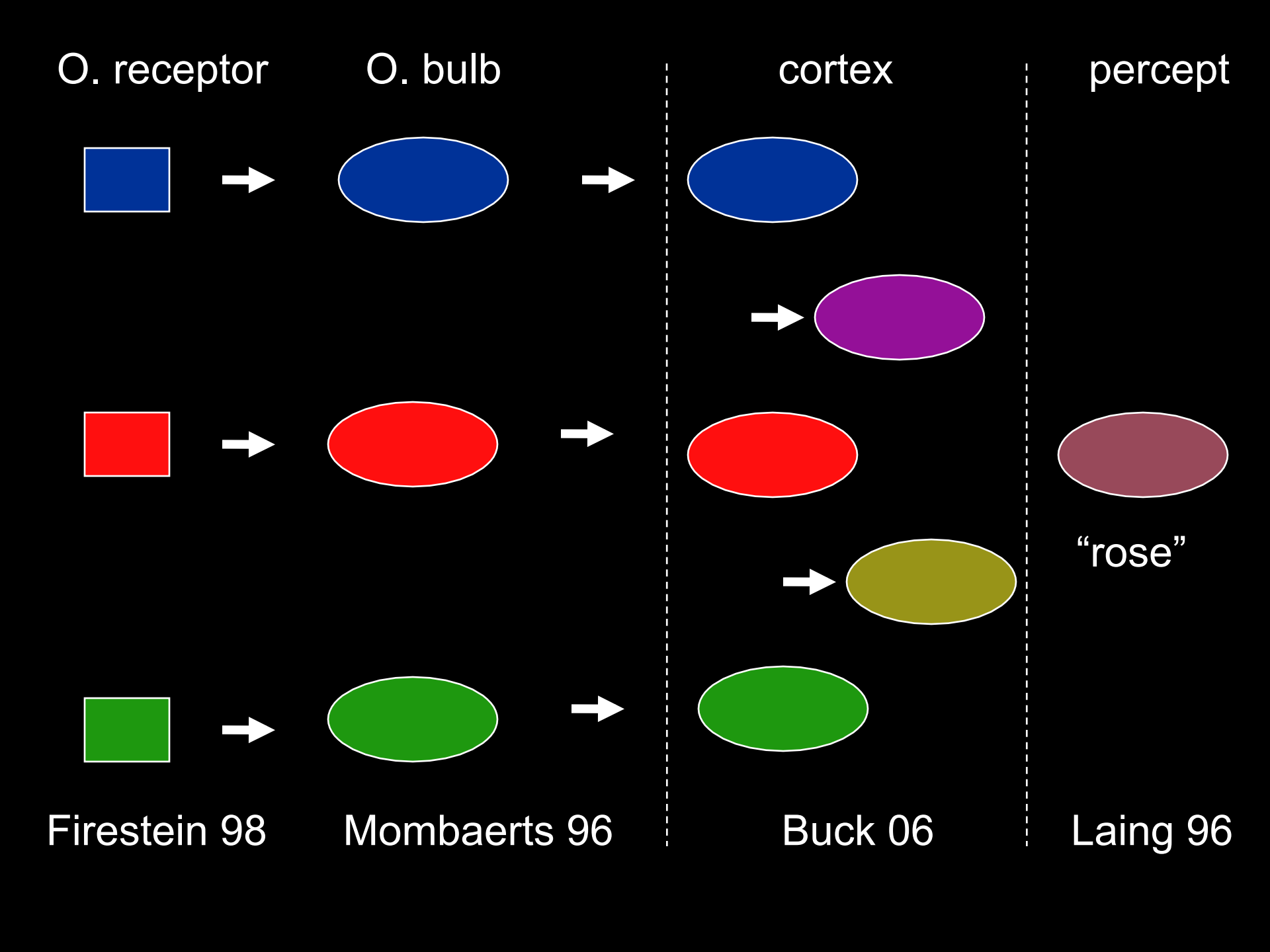
honey - cow dung - clove - something unnameable

Synthesis

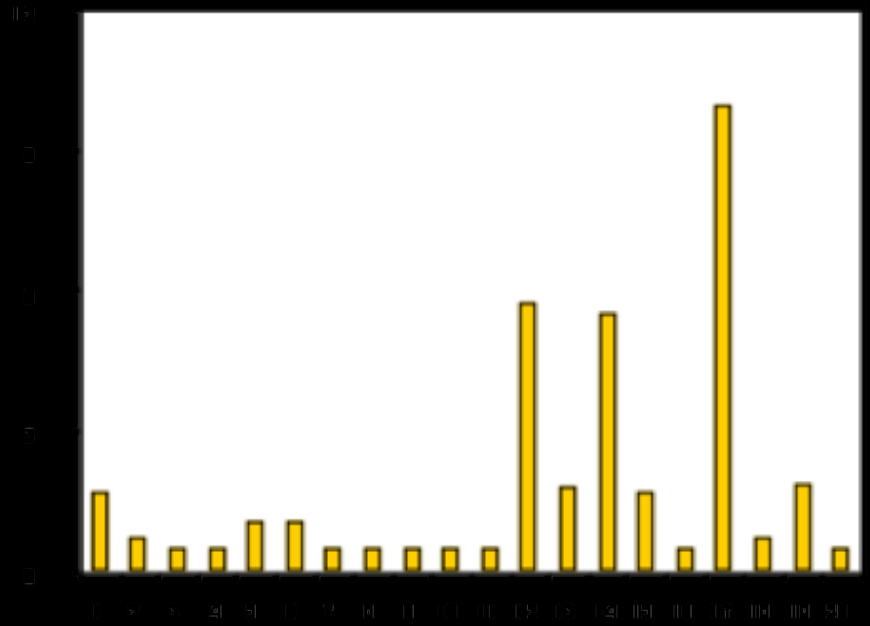


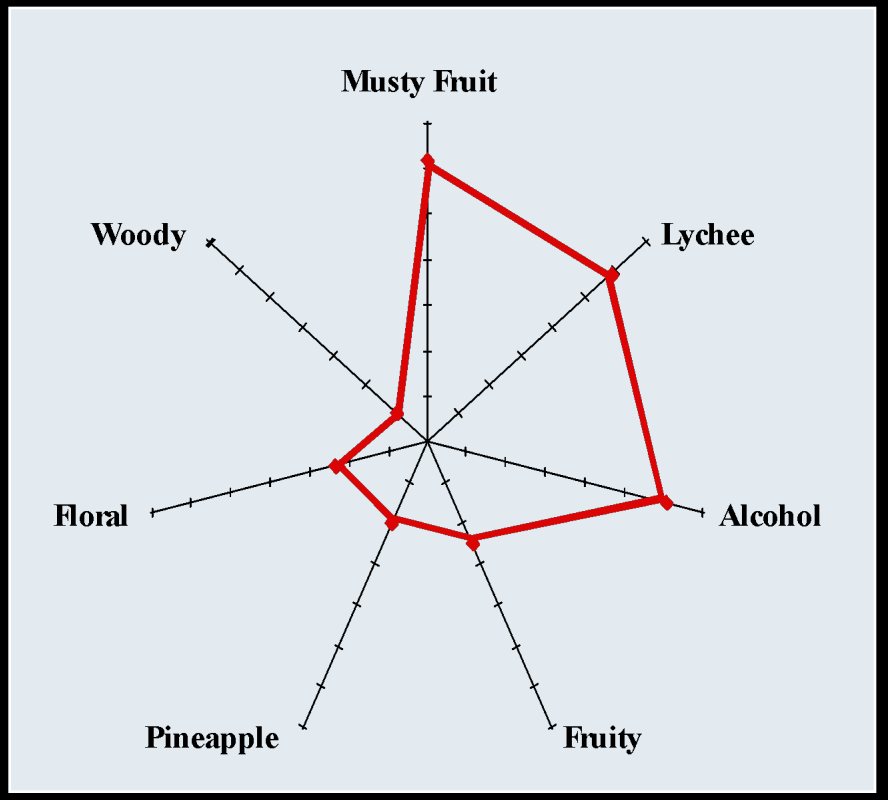
Mixture




O. receptor
O. bulb
cortex
percept
“rose”
Firestein 98
Mombaerts 96
Buck 06
Laing 96

Gewürztraminer wine





Descriptive Analysis of a model based of the Odor Spectrum

Odor Spectrum based on Guth ‘97

n-1 Omission Test

Lychee

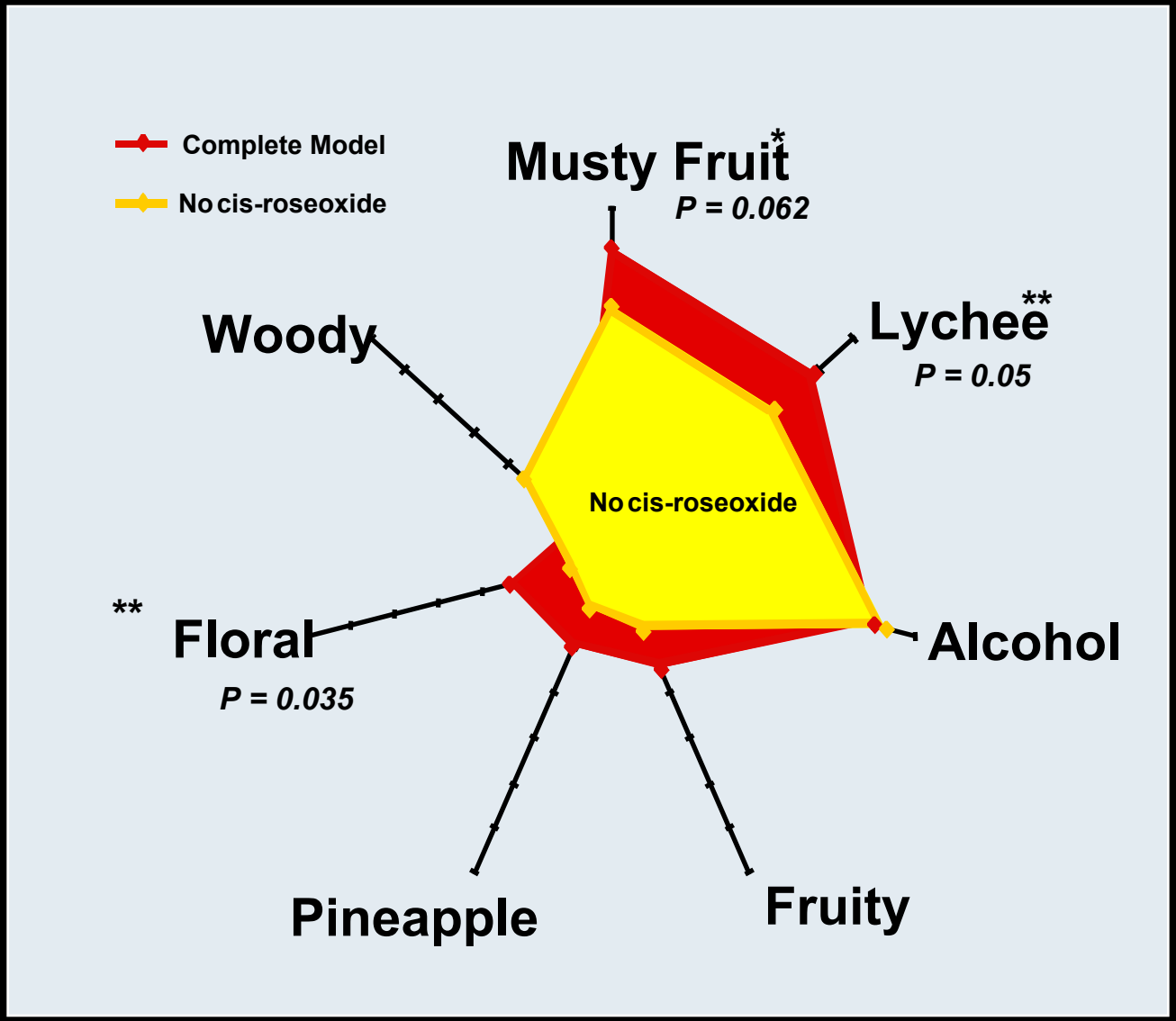
11.67

9.33

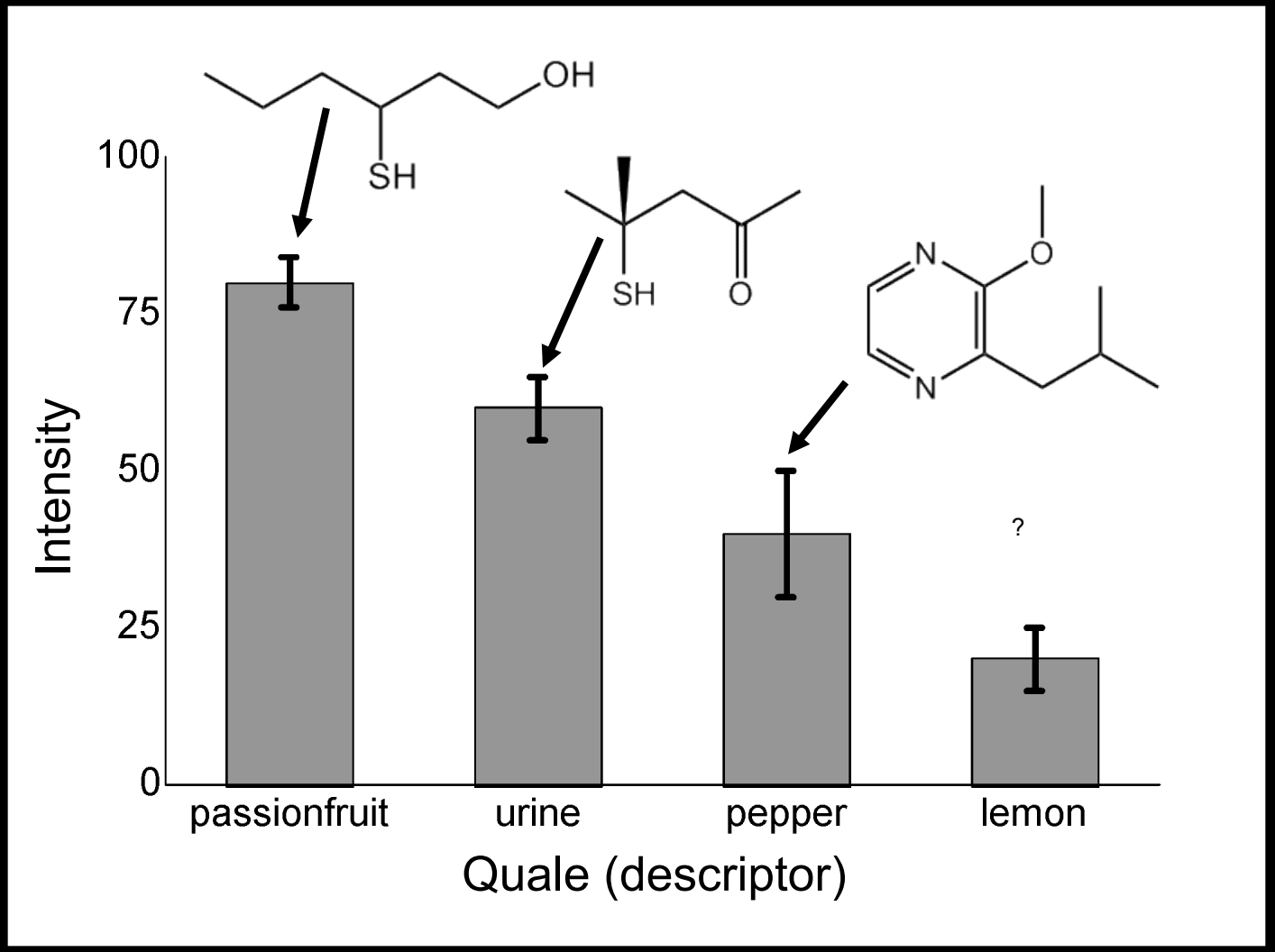
Floral

4.67

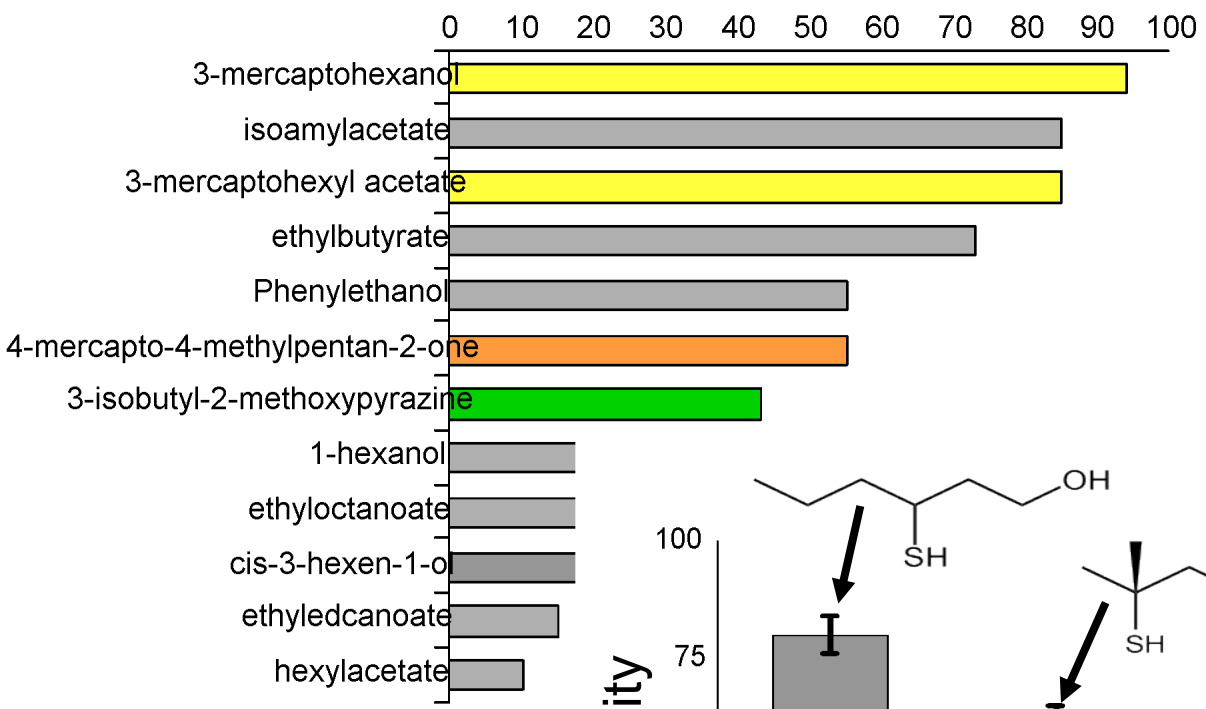
2.00



Sauvignon Blanc - Marlborough NZ

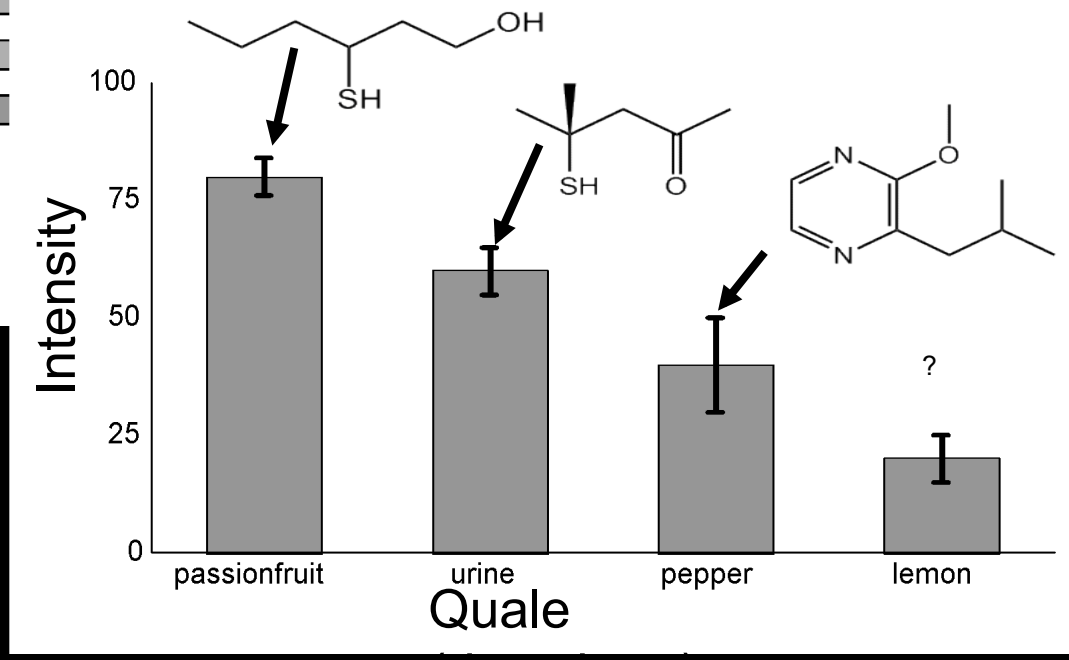


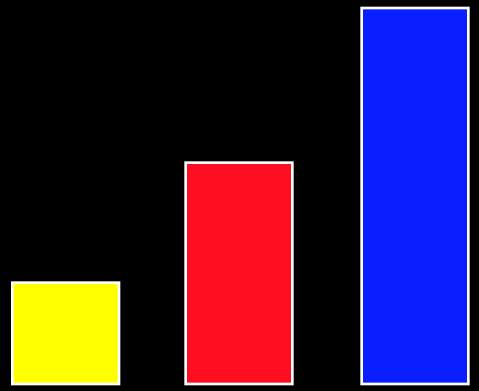
Brajkovich 05



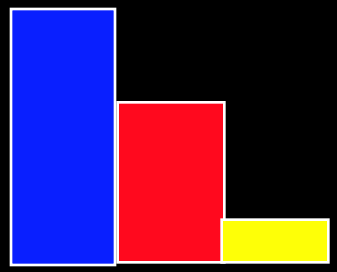
Determining the key aroma of New Zealand Sauvignon blanc wines.

L. NICOLAU,
F. BENKWITZ, T. TOMINAGA,
C. LUND and P. KILMARTIN



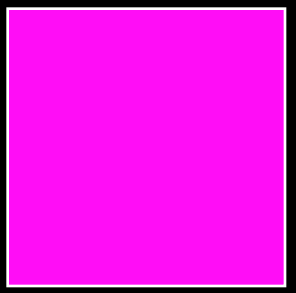


Mixture



clip

time ->



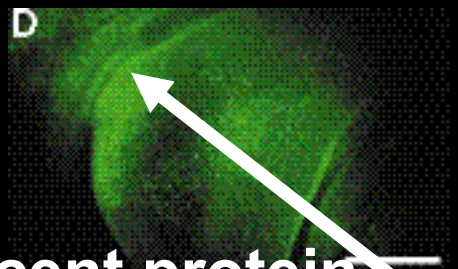
chimera

elemental
analytical
temporal

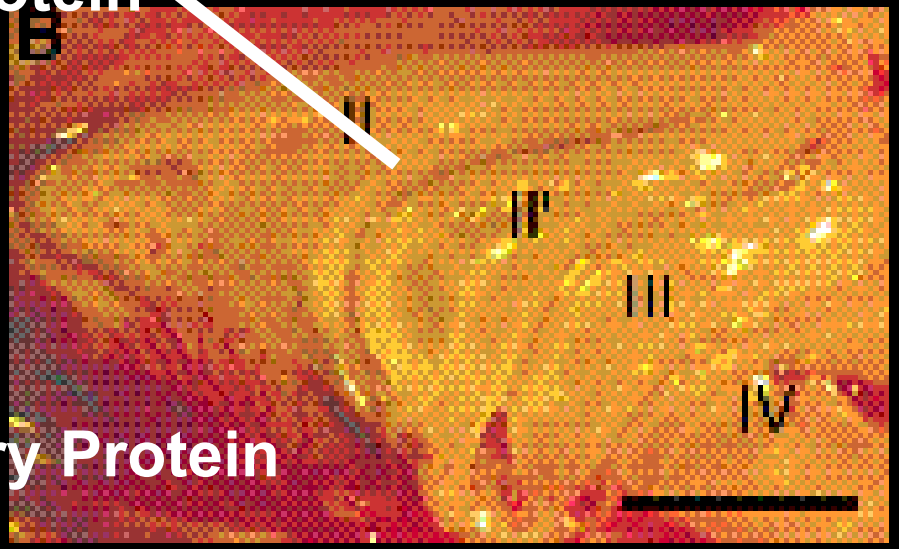
combinatorial
synthetic
assimilation

Functional Expression of Mammalian Odorant Receptor

Haiqing Zhao, Lidija Ivic, Joji M. Otaki, Mitsuhiro Hashimoto, Katsuhiro Mikoshiba, Stuart Firestein*



GFP - Green fluorscent protein



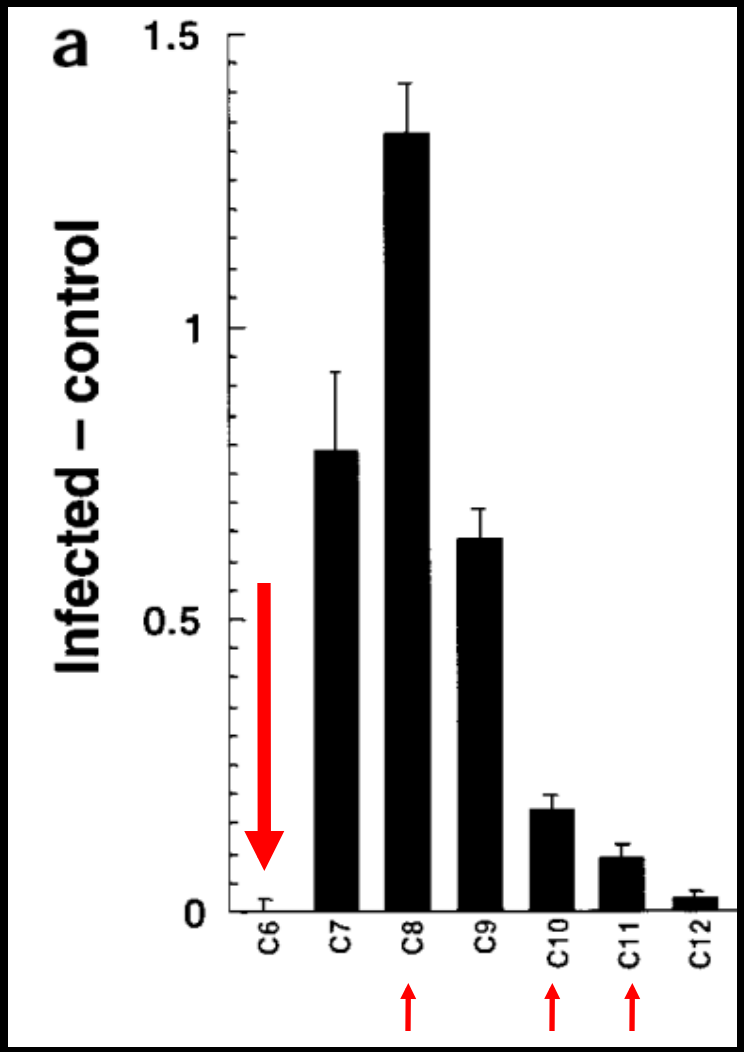
OR-I7 - Mammalian Olfactory Protein

Rat Olfactory Turbinate

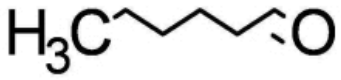
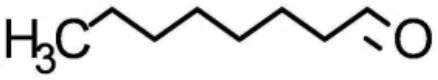
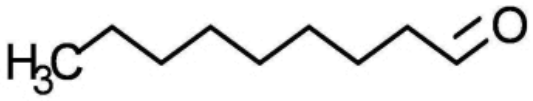
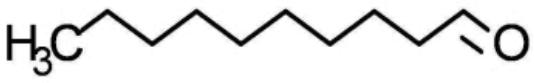
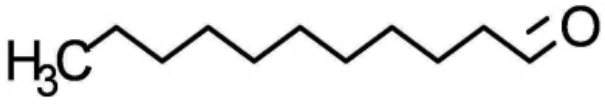
Zhao et al. 1998

Olfactory Receptor- OR I-7

- 1st OR paired with cognate ligand
- C_8 (Octanal) primary agonist
- EOG (electro-olfactogram) recordings
  - EOG interpreted as the summated generator potential of olfactory neurons.
  - Greatest number of neurons activated by C_8
- $C_7 \rightarrow C_{10}$ show greatest activation
- C_6 as antagonist (Peterlin et. al., 2008)



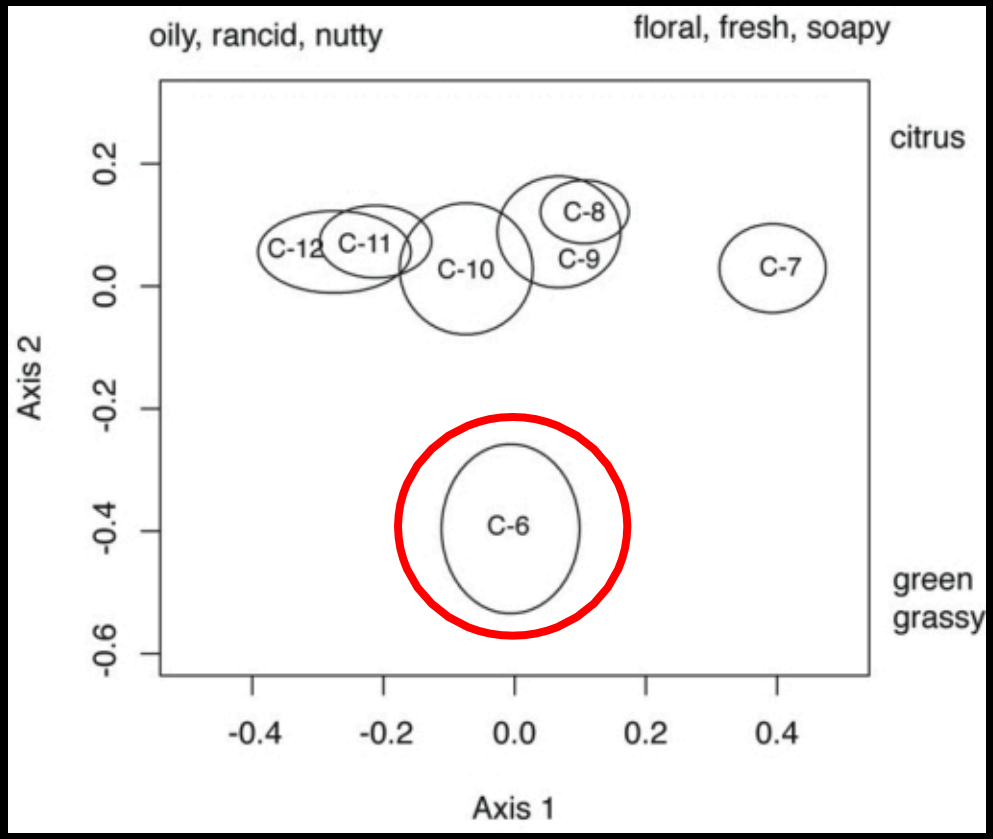
Araneda et. al. 2000.

Compound	Structure	CAS #	Molecular Weight	Odor Character	Detection Threshold
Hexanal (C_6)		66-25-1	100.1	Grass, tallow, fat	0.0045-5[a]; 0.00028[b]
Heptanal (C_7)		111-71-7	114.1	Fat, citrus, rancid	0.003[a]; 0.00018[b]
Octanal (C_8)		124-13-0	128.0	Fat, soap, lemon, green	0.0007[a]; 0.00001[b]
Nonanal (C_9)		124-19-6	142.1	Fat, citrus, green	0.001[a]; 0.00034[b]
Decanal (C_{10})		112-31-2	156.2	Soap, orange peel, tallow	0.0001-2[a]; 0.00040[b]
Undecanal (C_{11})		170-29	170.29	Oil, pungent, sweet	0.005[a]

* Published percepts listed on the Flavornet (Arn and Acree, 1998). [a]published detection thresholds ppm in water listed in Leffingwell et. al.[b] thresholds in ppm v/v listed in Nagata (1990).

Odor quality perception

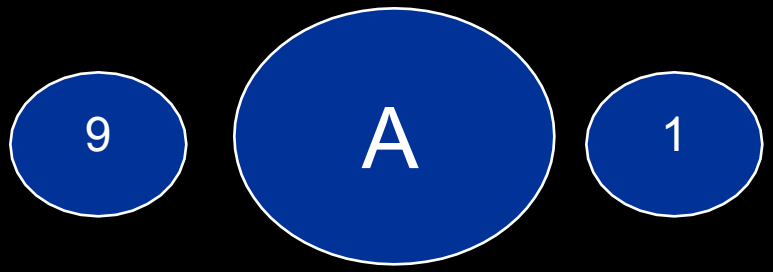
- Kittel et. al. (2008)
  - Free choice profiling C_6-C_{12}
- Procrustes analysis
  - C_6 = Different!!
- Confirmed
  - C_6=Green odor
  - C_7-C_9 = Citrus
  - C_{10}-C_{12} = Nutty/ Rancid

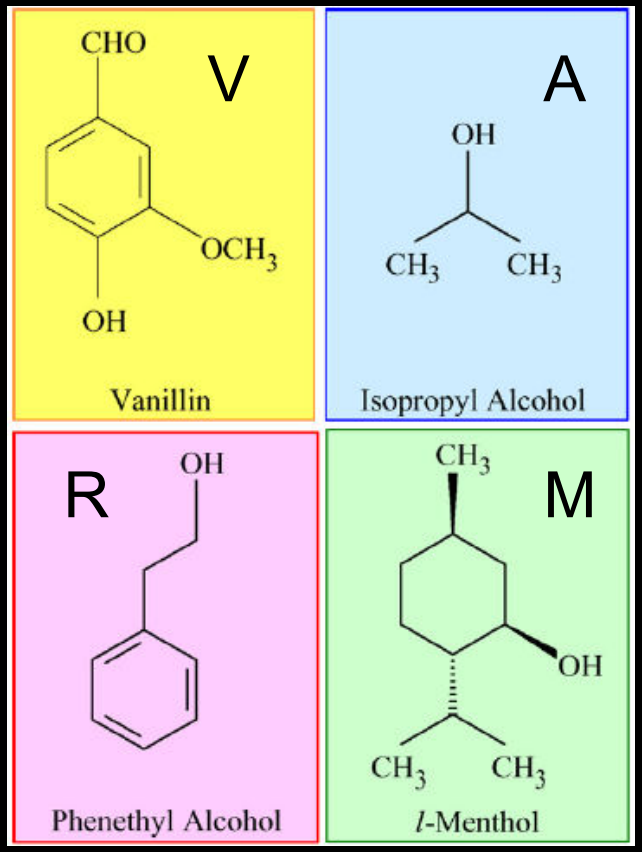


Kittel (2008)

Adaptation

- Delivery method :
- Polyethylene bottles with Teflon balls
- Strips changed daily





Vanilla (V)		Alcohol (A)	
Adapt	***Test***	*Adapt*	Test
W	**V**	W	**A**
A	**VA**	V	**VA**
R	**VR**	R	**AR**
M	**VM**	M	**AM**
AR	**VAR**	VR	**VAR**
AM	**VAM**	VM	**VAM**
RM	**VRM**	RM	**ARM**
ARM	**VARM**	VRM	**VARM**

Rose (R)		Mint (M)	
Adapt	***Test***	*Adapt*	Test
W	**R**	W	**M**
V	**VR**	V	**VM**
A	**AR**	A	**AM**
M	**RM**	R	**RM**
VA	**VAR**	AR	**ARM**
AM	**ARM**	VA	**VAM**
VM	**VRM**	VR	**VRM**
VAM	**VARM**	VAR	**VARM**

"Characteristic component odors emerge from mixtures after selective adaptation." Holly F. Goyert, Marion E. Frank , Janneane F. Gent , Thomas P. Hettinger

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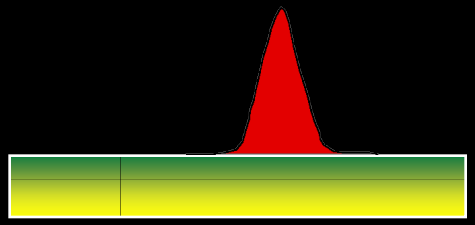
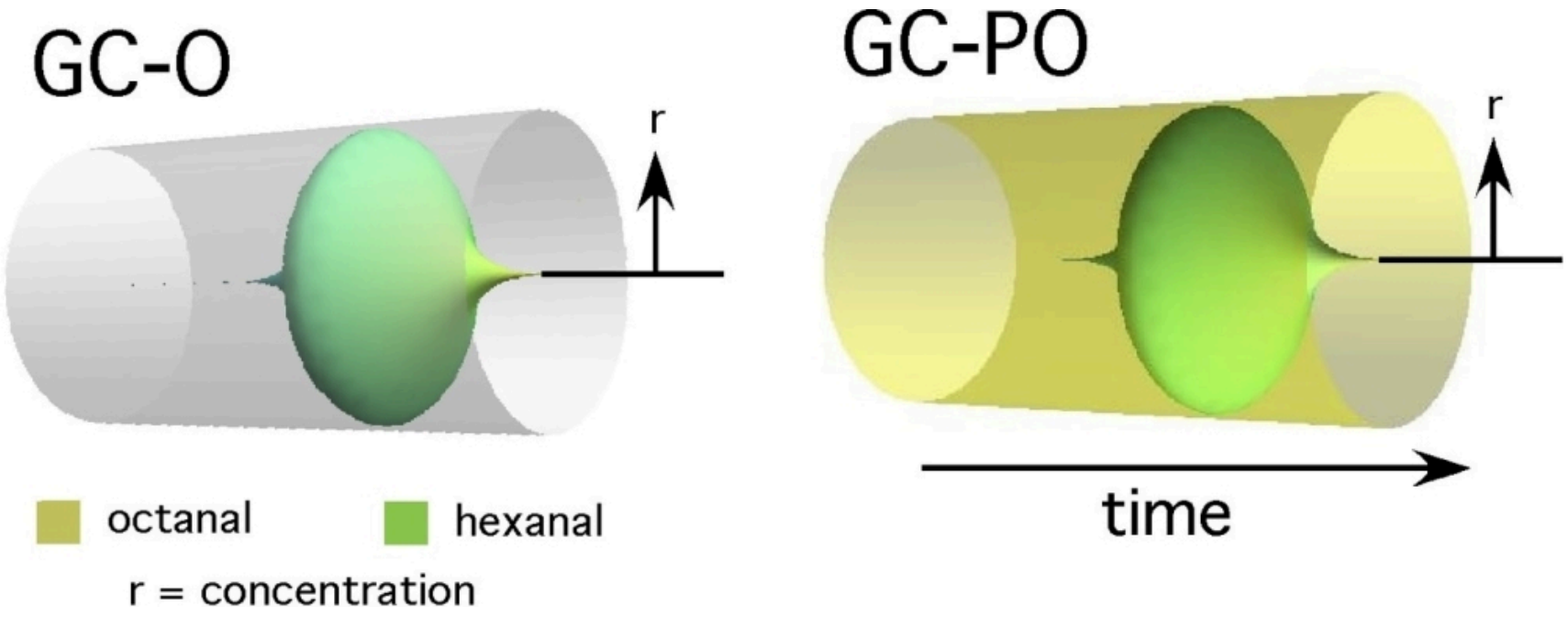
Pedestal GC Olfactometer



hexanal

octanal

undecanal

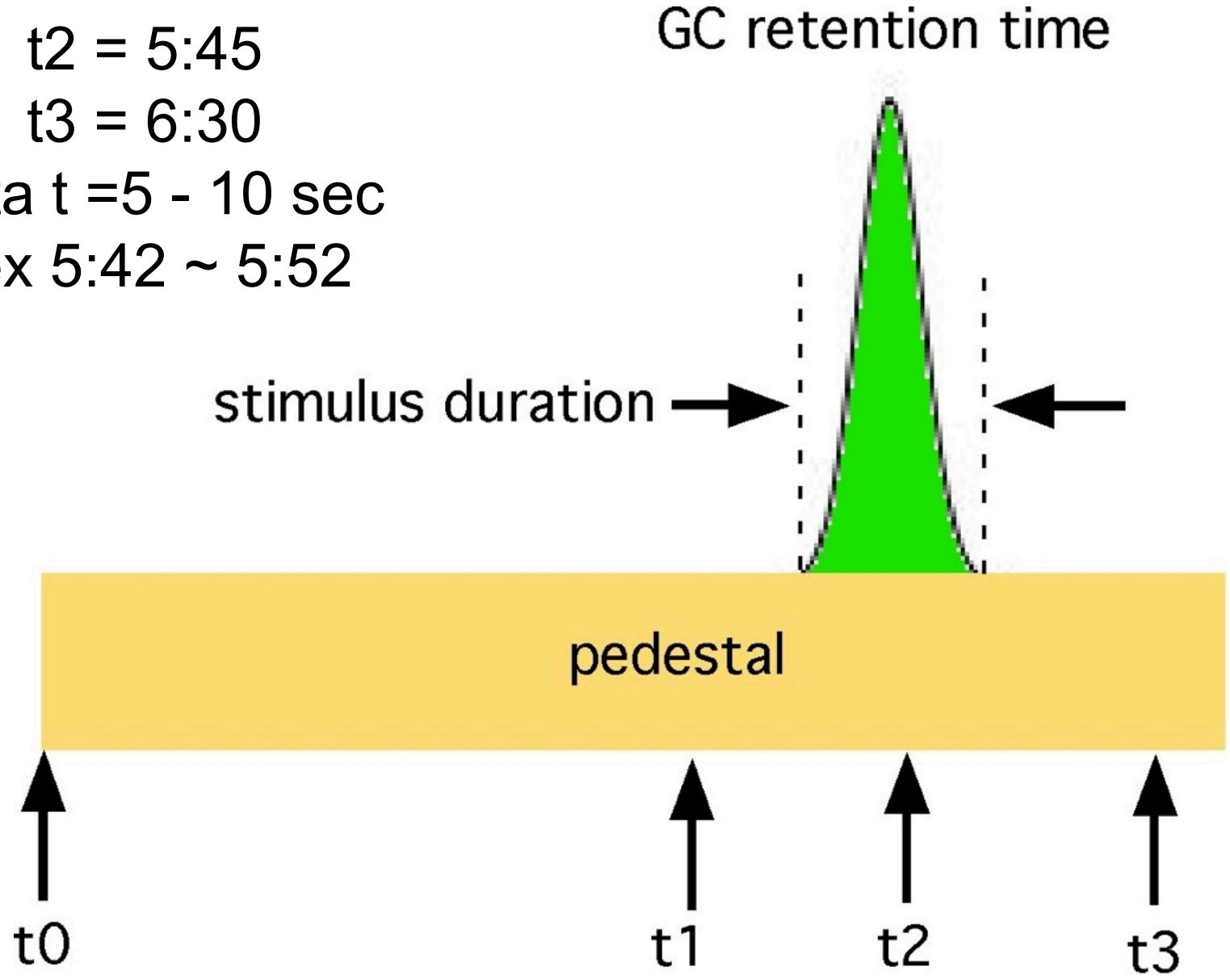

GC-O
r
GC-PO
r
octanal
hexanal
r = concentration
time

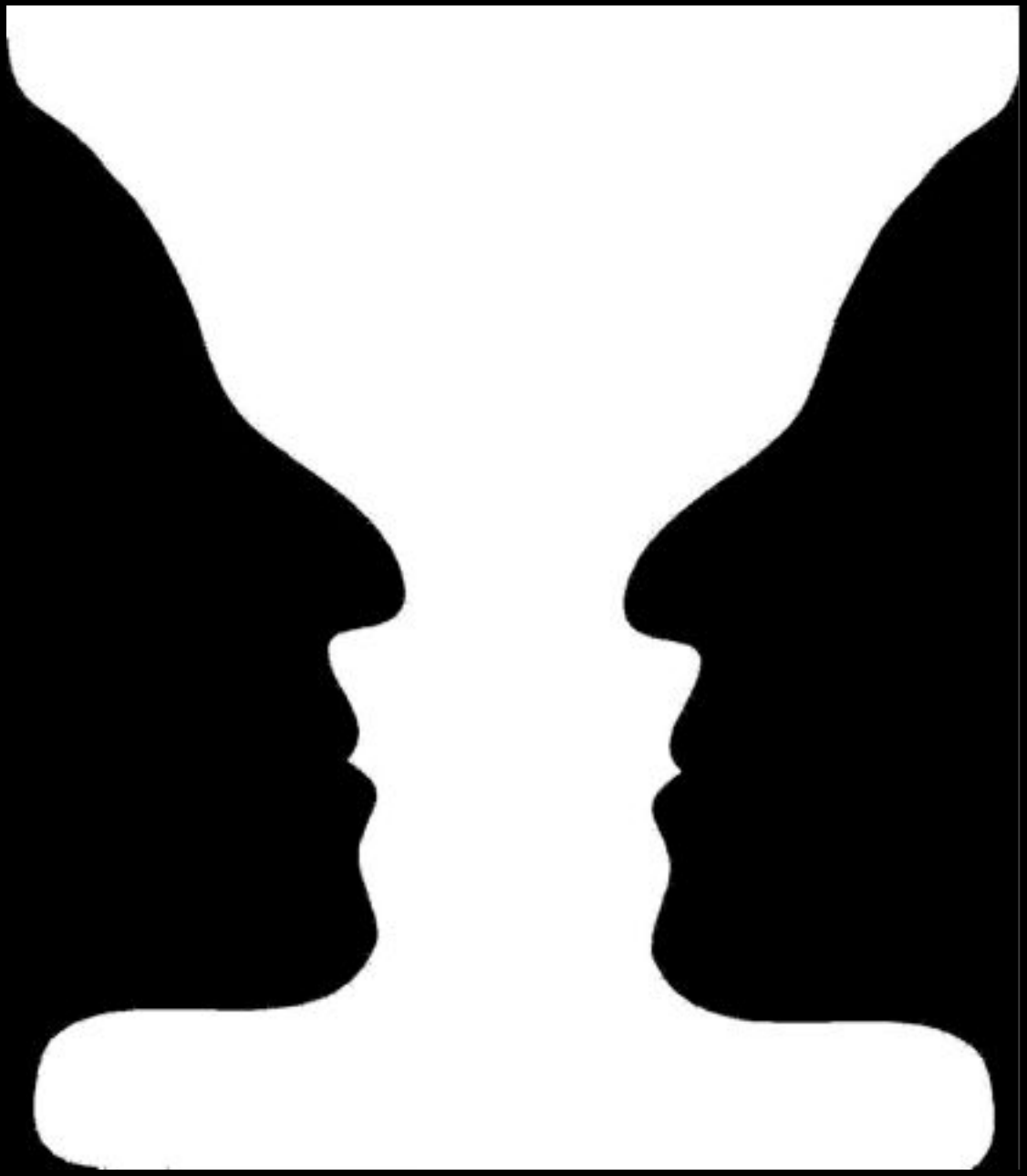
t2 = 5:45

t3 = 6:30

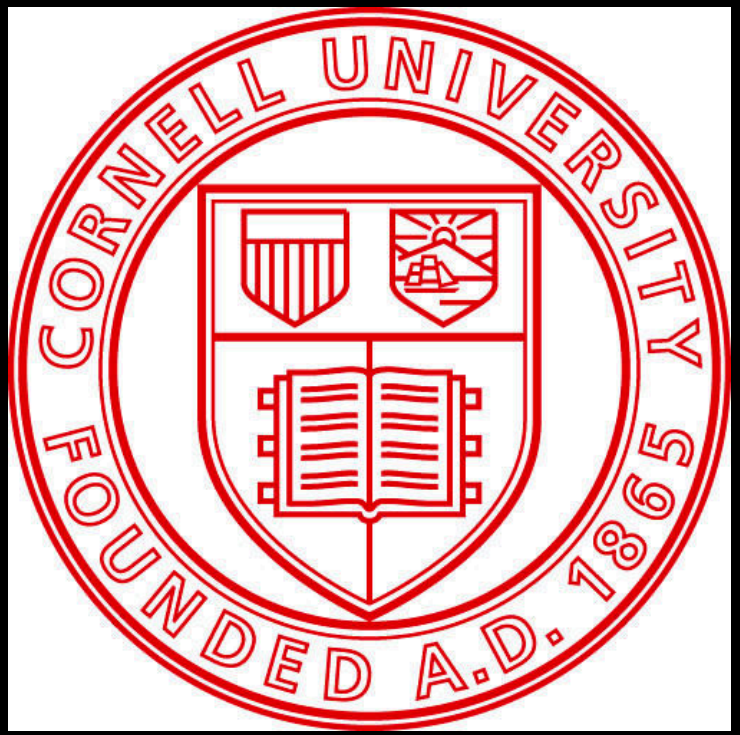
delta t =5 - 10 sec

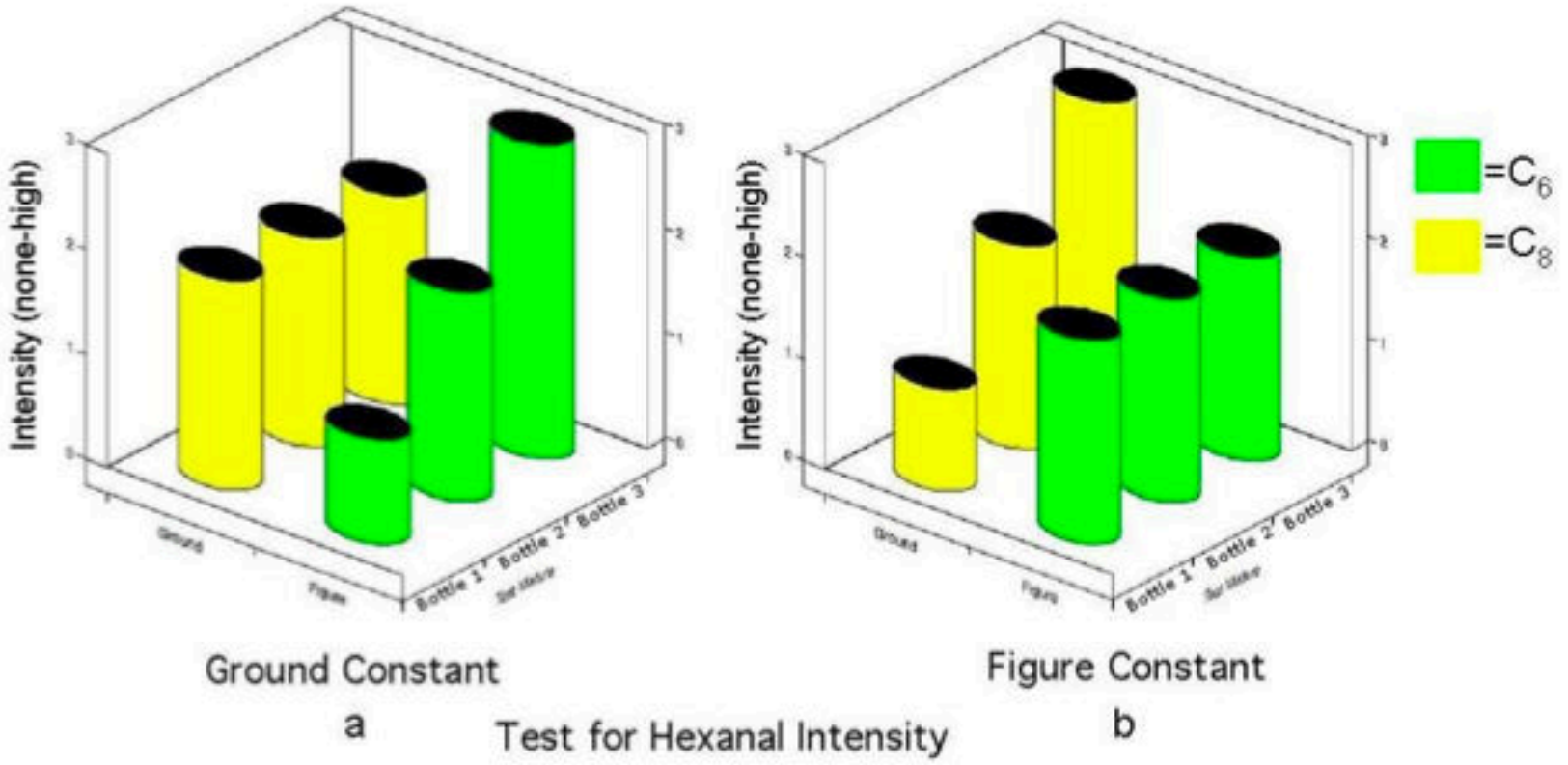
hex 5:42 ~ 5:52





Fin…





Ground Constant

a

Test for Hexanal Intensity

Figure Constant

b

What does chemical knowledge tell us?

The dots and dabs