

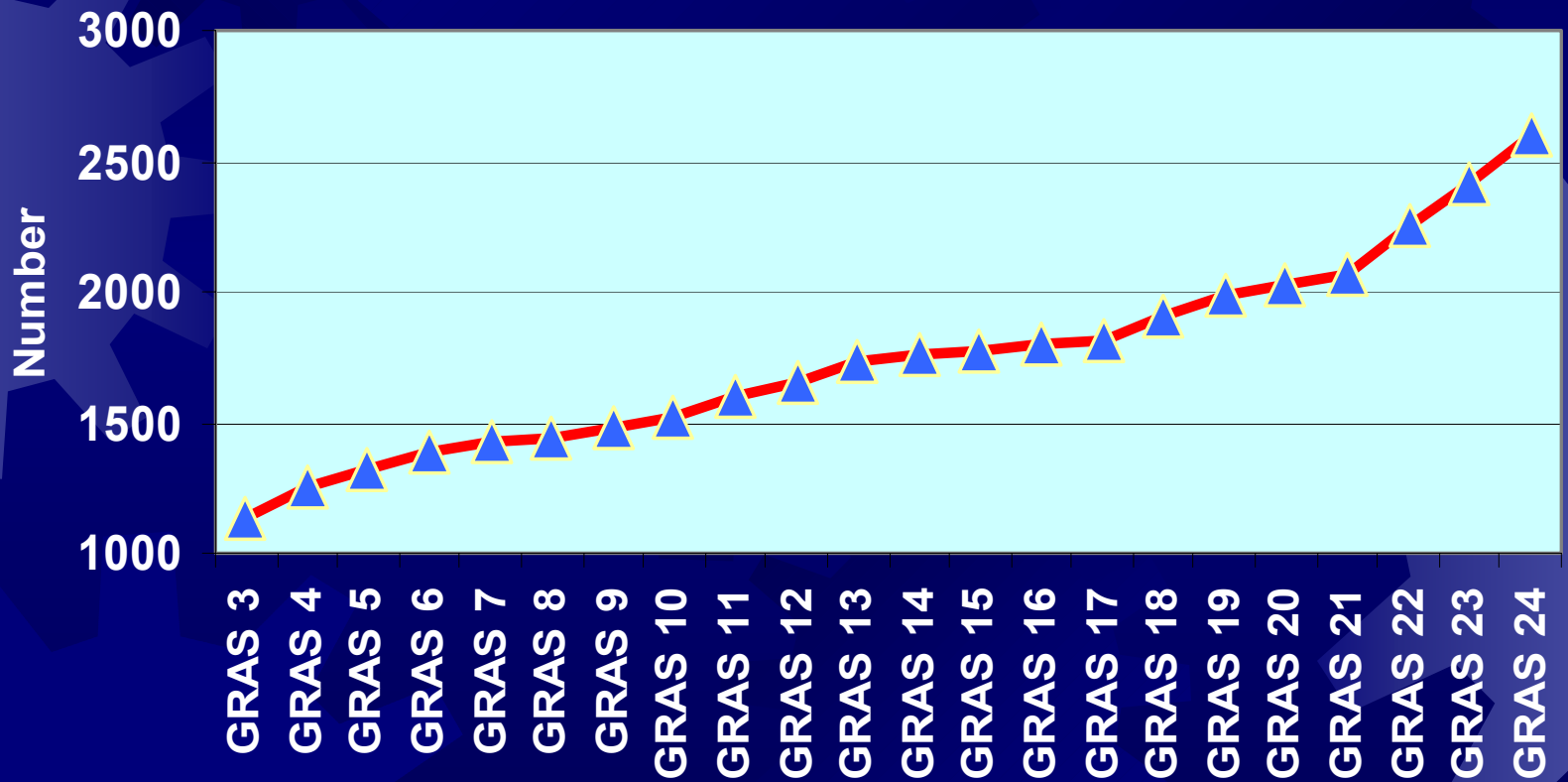
Odds & Trends in F&F – Technical Evolution & Information Revolution



John C. Leffingwell
Society of Flavor Chemist's
November 20, 2008

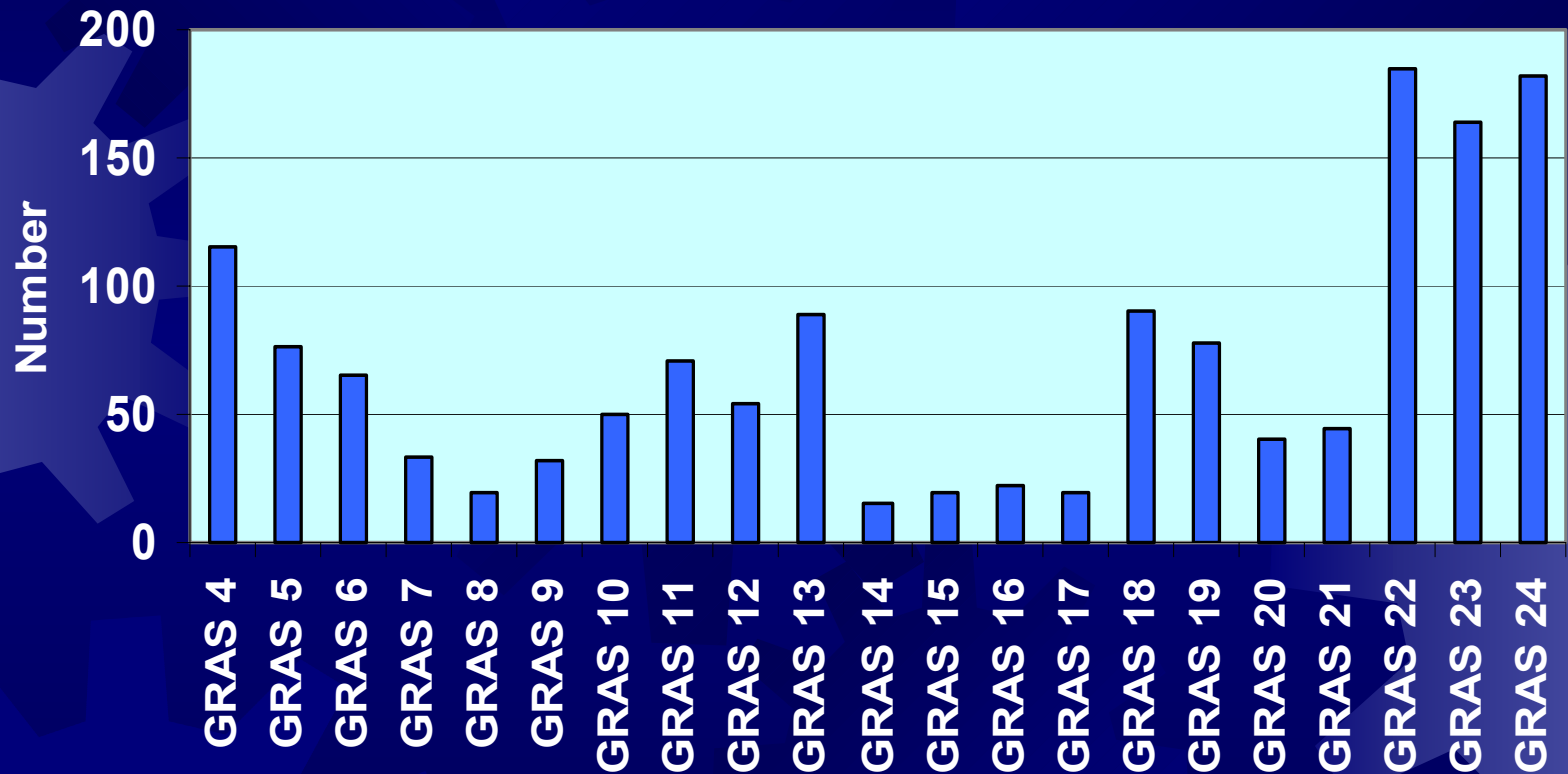
Additions to Original GRAS List

Cumulative Number of GRAS Items



Additions to Original GRAS List

Number of GRAS Items



20+ % from GRAS 22, 23 and the forthcoming GRAS 24

Technical Evolution of the F&F Industry

- 50's to 80's – Instrumentation - IR, NMR, GC-MS
- 90's to Present – Application of Drug design techniques, SAR, Biotechnology, Genomics
- Today's Examples:
 - Receptor gene expression & ligand (agonist) screening for new potent tastants, flavor modifiers, cooling agents, sweetness enhancers, etc.
 - Methodology – Fluorescent Calcium Imaging (EC_{50}) to measure a ligands potency against a receptor

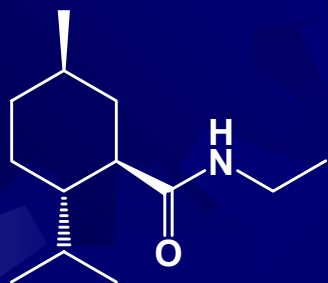
Thermo TRP Receptors & Agonists

Table 4 Thermoreceptor Agonists

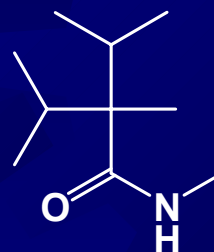
Chemical agonist (botanical source)	ThermoTRP
Capsaicin (hot chilli peppers, e.g., Tabasco)	TRPV1
Piperine (black pepper corns)	TRPV1
Allicin (fresh garlic)	TRPV1, TRPA1
Camphor (Cinnamomum camphora)	TRPV3, TRPV1
D-9-Tetrahydrocannabinol (Cannabis sativa)	TRPV2, TRPA1
2-Aminoethoxydiphenyl borate (synthetic)	TRPV1, TRPV2, TRPV3
4-a-phorbol 12,13-didecanoate (synthetic)	TRPV4
(-)-Menthol (peppermint)	TRMP8, TRPV3
1,8-Cineole, eucalyptol (eucalyptus)	TRPM8
WS-3 (synthetic)	TRPM8
Icilin (synthetic)	TRPM8, TRPA1
Cinnamaldehyde (cinnamon, cassia)	TRPA1, TRPV3
Allyl isothiocyanate (mustard, horseradish)	TRPA1
Benzyl isothiocyanate (mustard, horseradish)	TRPA1
Phenethyl isothiocyanate (mustard, horseradish)	TRPA1

Leffingwell, Handbook of Cosmetic Science and Technology, 3d edition (2009), In Press

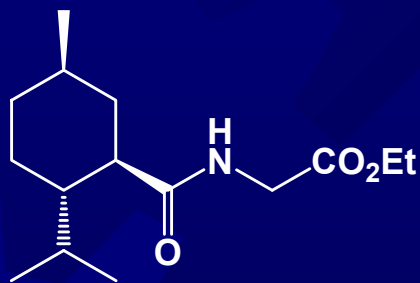
Amide GRAS Cooling Agents Thru GRAS 23



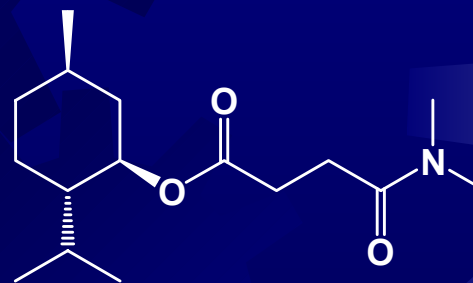
WS-3
FEMA 3455
1.5 X Menthol



WS-23
FEMA 3804
0.75 X Menthol

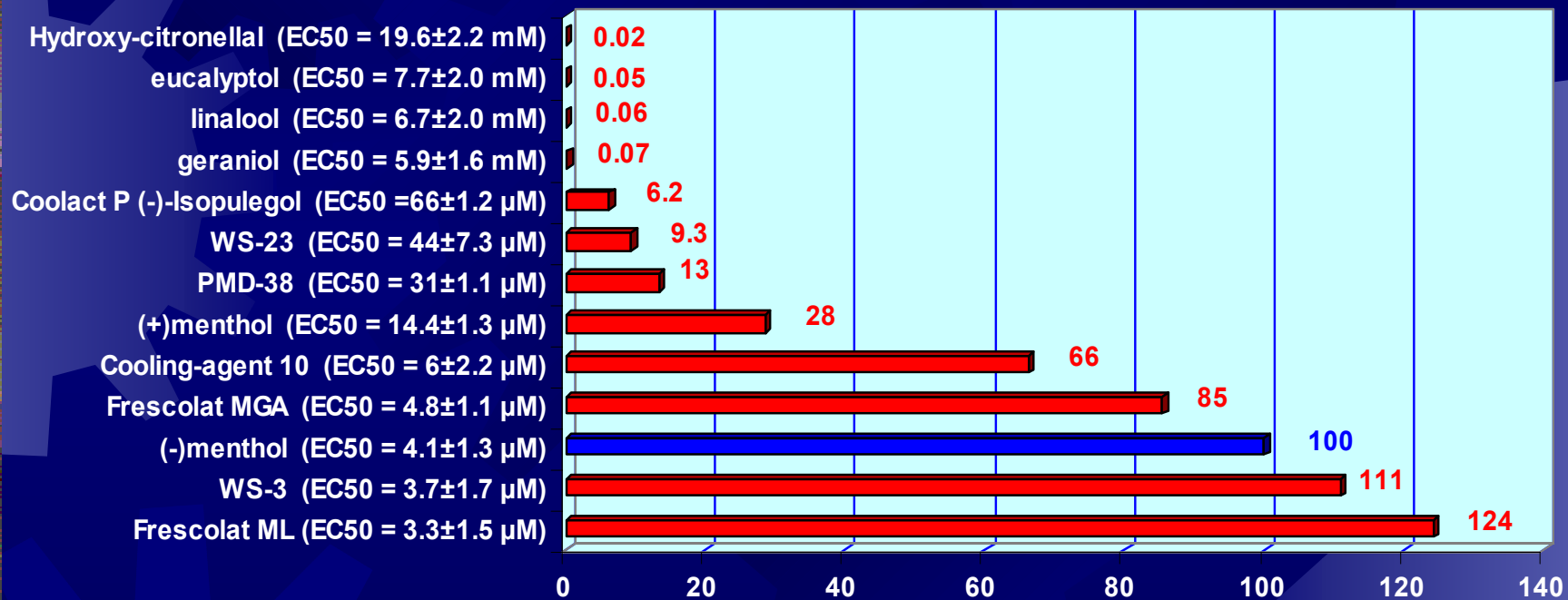


WS-5
FEMA 4309
4 X Menthol



Menthyl N,N-dimethylsuccinamide
FEMA 4230

Relative Potency of TRPM8 agonists based on EC₅₀ values (mean) with (-)-Menthol = 100



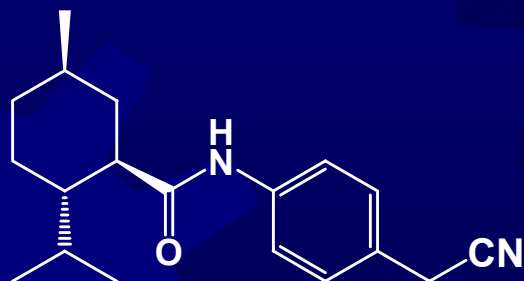
Note - Icilin (EC₅₀ = 0.2 ± 0.1 μM) not shown
 (Relative icilin potency vs (-)-Menthol at 100 is 2050) - Adapted
 from Behrendt, et .al, Brit. J. Pharm., 141:737-745 (2004)

Givaudan's New Powerful GRAS Cooling Agents

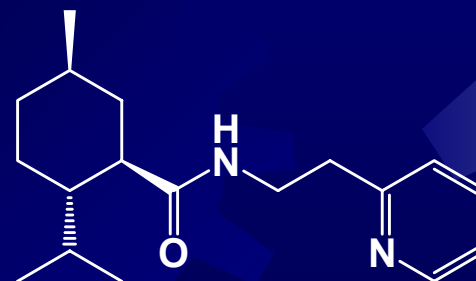
Table 1 Comparison of data for the TRPM8 activation, expressed as EC₅₀ and iso-intensity to menthol of selected menthane carboxamides

Cpd.	R ₁	R ₂	EC ₅₀ (μM)	Isointensity (ppm)	CAS no.
2a	CH ₃	CH ₃	25.6	2.0	39668-77-4
2b	C ₂ H ₅	H	3.6	1.5	68489-00-9
2c	CH ₂ C ₆ H ₅	H	3.5	2.0	73435-72-0
2d	4-C ₆ H ₄ SO ₂ NH ₂	H	0.7	0.5	852379-29-4
2e	C ₆ H ₅	H	0.6	1.0	824947-52-6
2f	2-C ₆ H ₄ CONH ₂	H	0.6	0.5	915962-26-4
2g	4-C ₆ H ₄ OCH ₃	H	0.5	2.0	68489-09-8
2h	4-C ₆ H ₄ CONH ₂	H	0.4	0.15	847564-94-7
2i	4-C ₆ H ₄ CH ₂ OH	H	0.4	1.0	847564-90-3
2j	4-C ₆ H ₄ CH ₂ CN	H	0.2	0.2	852379-28-3
2k	CH ₂ CH ₂ (2-C ₅ H ₄ N)	H	0.1	0.05	926913-58-8
2l	2-C ₆ H ₅ OCH ₃	H	5.1	2.0	824947-60-6
2m	CH ₂ CH ₂ CH ₂ OCH(CH ₃) ₂	H	0.9	0.7	663218-92-6

Furrer et al., Chem. Percept. (July 2008) 1:119–126; Galopin et al., US Patent 7,414,152 (August 19, 2008); Bell et al., WO2007019719 (Feb. 22, 2007)

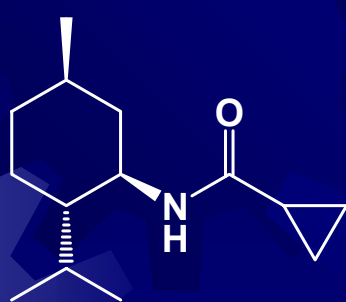


2j = FEMA 4496
10X Menthol

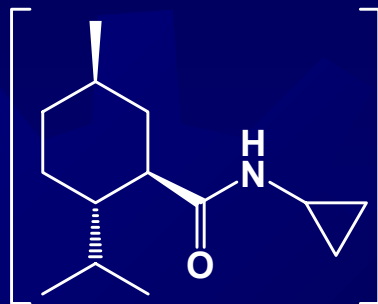


2k = FEMA 4549
40-100X Menthol

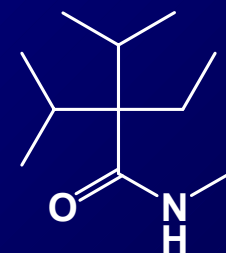
New GRAS 24 Cooling Agents



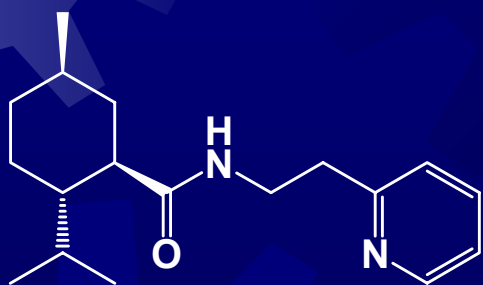
or



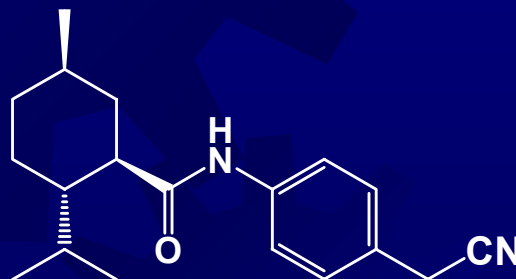
Menthyl
cyclopropanecarboxamide
FEMA 4558



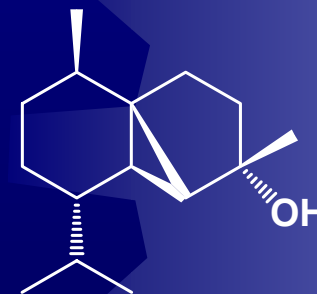
N-Ethyl-2,2-diisopropyl-
butanamide
FEMA 4557



N-(2-(Pyridin-2-yl)ethyl)-3-p-
menthanecarboxamide
FEMA 4549
40-100 X Menthol

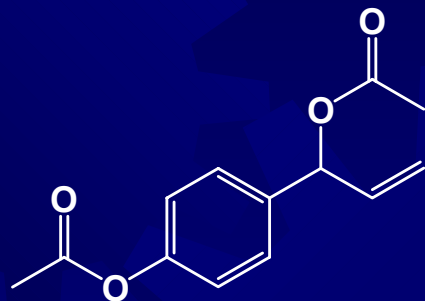


N-p-Benzeneacetonitrile-
menthanecarboxamide
FEMA 4496
10 X Menthol



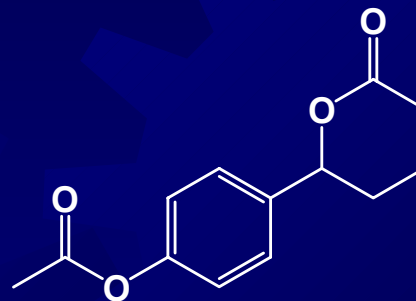
Cubebol
FEMA 4497

New GRAS Warming / Pungent Agents



Galangal acetate

**Not GRAS but Galangal extracts are
Yang & Eilerman, J. Agric. Food
Chem. 1999, 47, 1657-1662**



Dihydrogalangal acetate

**FEMA 4555
Bachmann et al. EP1700525**

Wasabi-like GRAS 23 Warming / Pungent Agents

Erucin – FEMA 4414

Lesquerellin – FEMA 4415

Berteroin – FEMA 4416

Amyl isothiocyanate – FEMA 4417

3-Butenyl isothiocyanate – FEMA 4418

sec-Butyl isothiocyanate – FEMA 4419

Ethyl isothiocyanate – FEMA 4420

5-Hexenyl isothiocyanate – FEMA 4421

Hexyl isothiocyanate – FEMA 4422

Isoamyl isothiocyanate – FEMA 4423

Isobutyl isothiocyanate – FEMA 4424

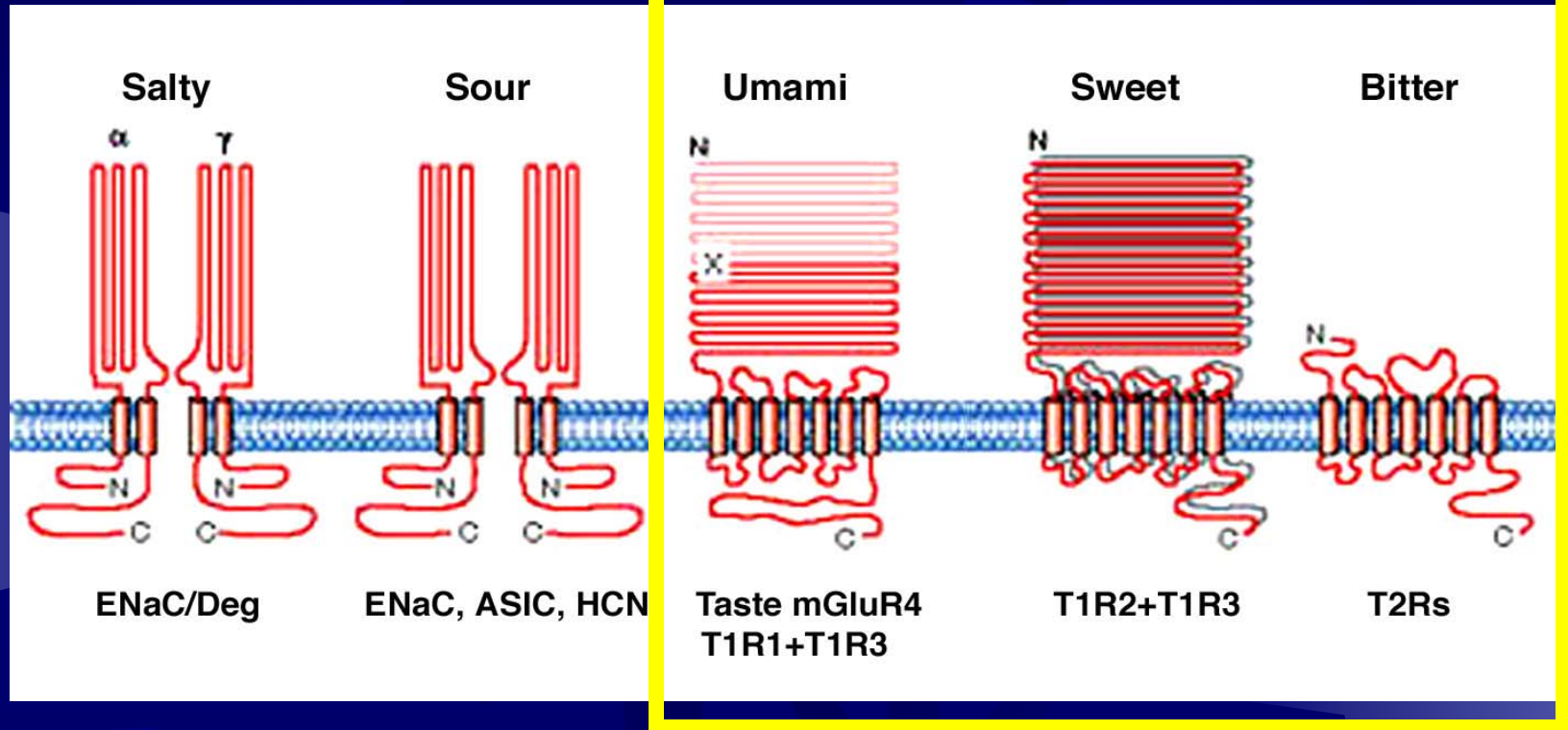
Isopropyl isothiocyanate – FEMA 4425

Methyl isothiocyanate – FEMA 4426

4-pentenyl isothiocyanate – FEMA 4427

Benzyl isothiocyanate – FEMA 4428

Taste Receptors



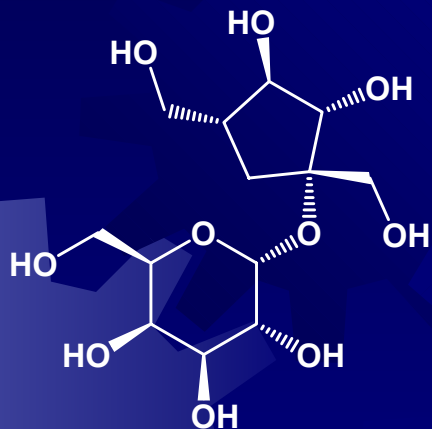
Lindemann, *Nature* 413: 219-225 (2001)

Salt & Sour Receptors are Ion Channels

Umami, Sweet & Bitter Receptors are GPCR Receptors

For examples (sweet and umami) - See Li et al., *PNAS*, 2002, 99 (7) 4692-4696

Diverse Compounds are Sweet



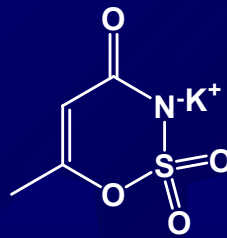
Sucrose



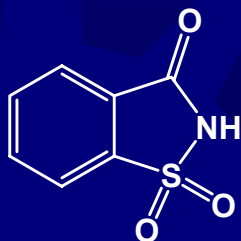
Sucralose



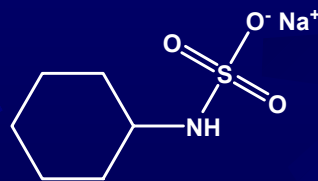
Aspartame



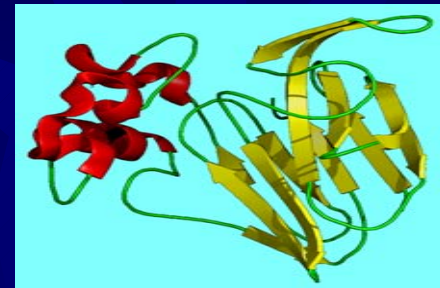
Acesulfame K



Saccharin



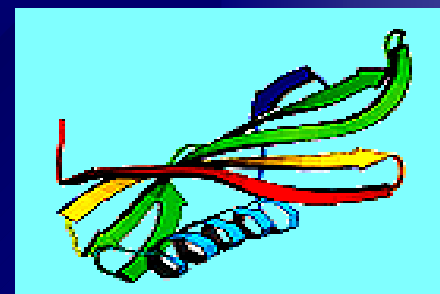
Cyclamate



Thaumatin

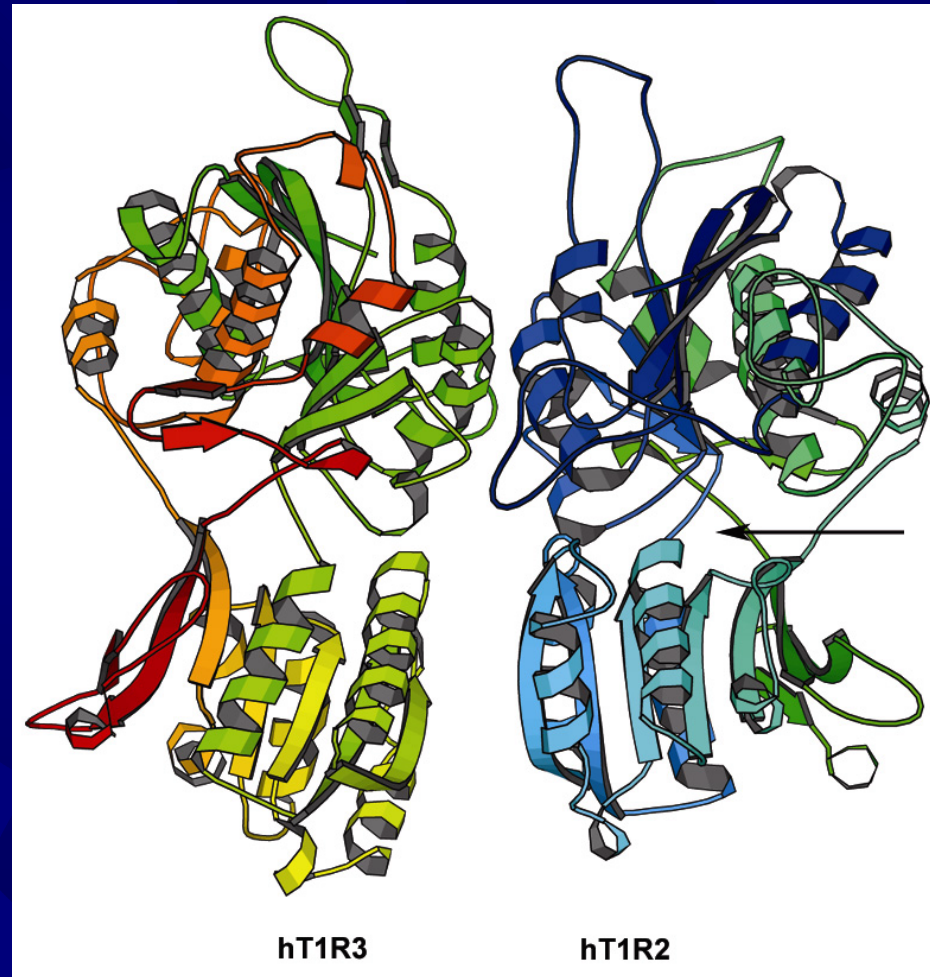


Brazzein



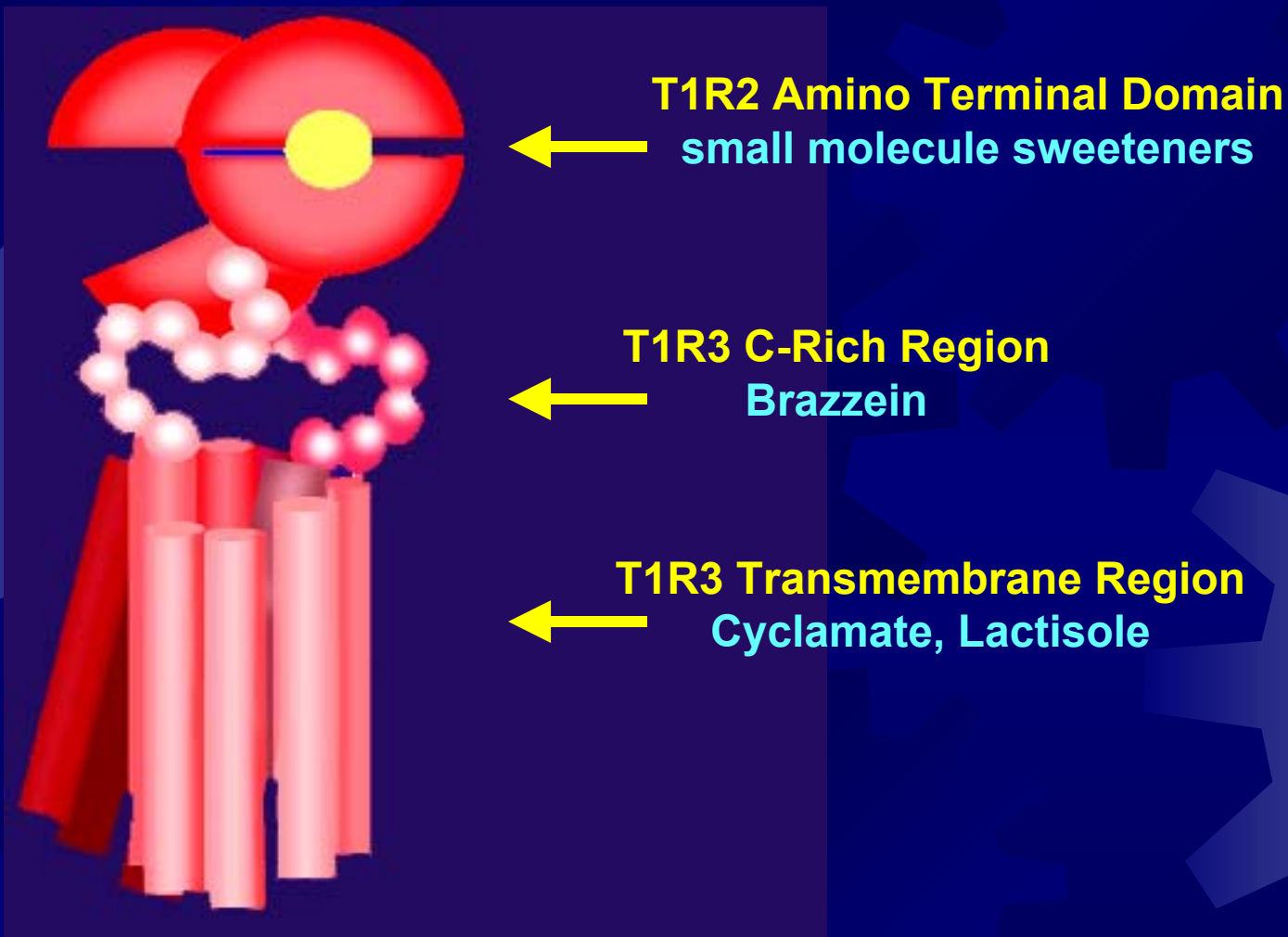
Monellin

Multiple Regions of T1R2+T1R3 are Required for Effective Interaction with Different Sweet Compounds



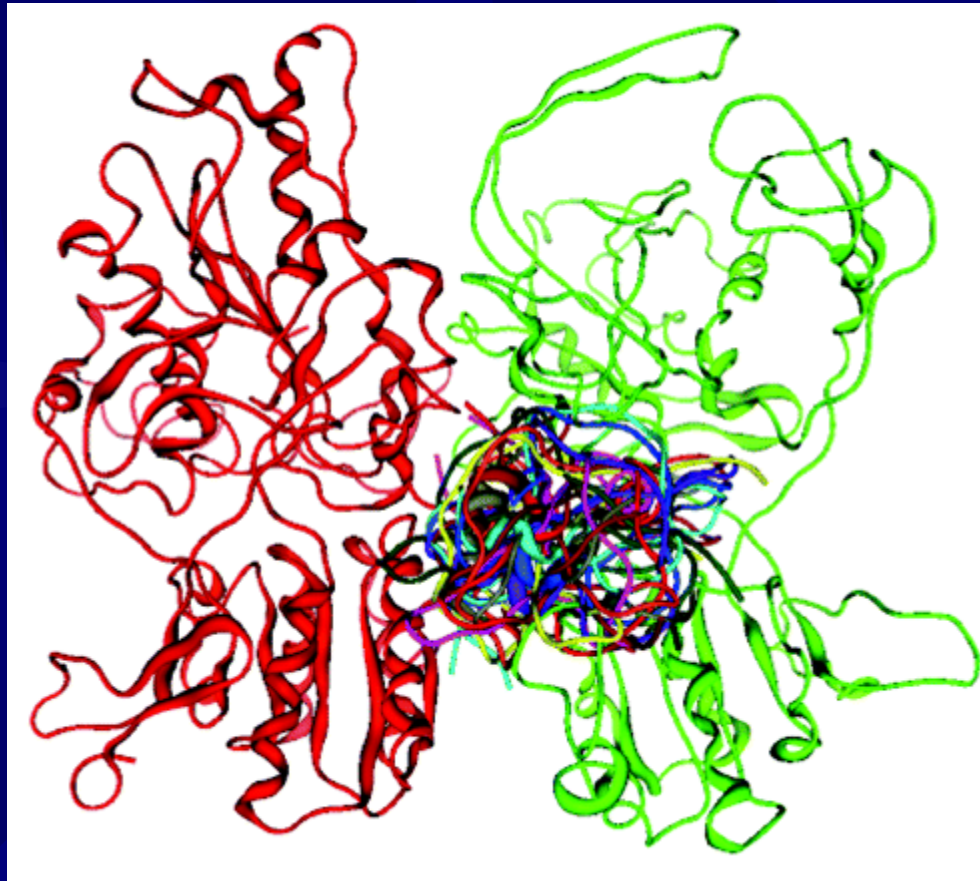
R. F. Margolskee, *Sci. STKE*, 28 June 2005

Multiple Regions of T1R2+T1R3 are Required for Effective Interaction with Different Sweet Compounds



R. F. Margolskee, *Sci. STKE*, 28 June 2005

Sweet Protein Brazzein Docked to the T1R3 Subunit



Walters et al., *J Agric Food Chem.* 2006; 54(26): 10129–10133

Synomyx Sweetness Enhancers

November 5, 2008 – Senomyx receives GRAS status for **S2383** – an enhancer that allows a 75% reduction of Sucralose

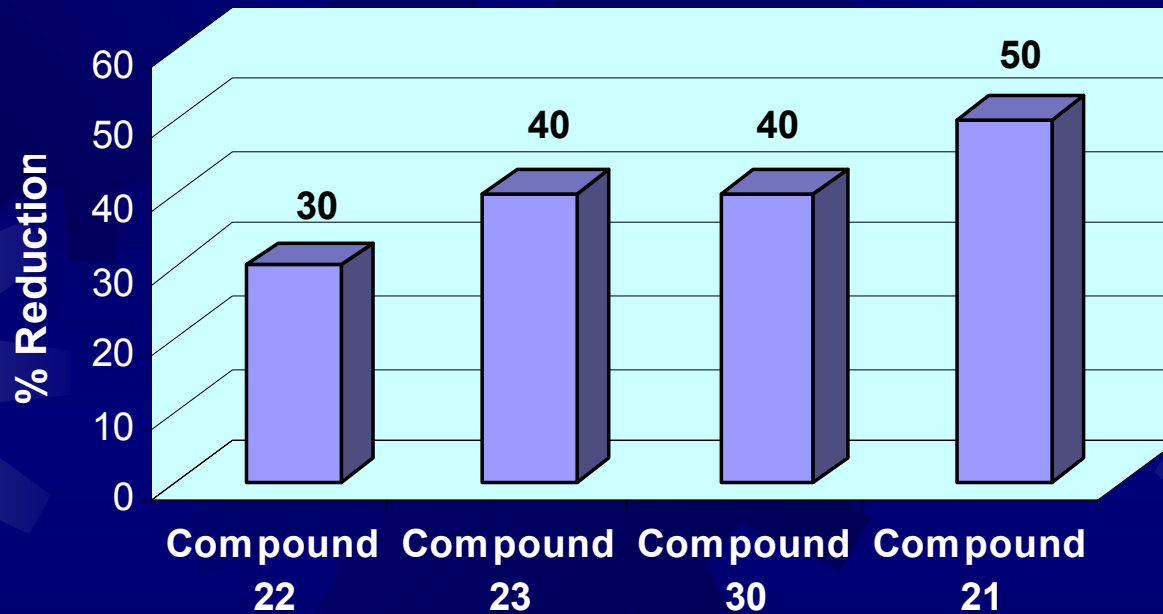
November 6, 2008 – Senomyx enters a collaborative commercialization and license agreement with Firmenich for **S2383**

Senomyx has also initiated development activities for **S6973**, a new sucrose enhancer that enables up to a 50% reduction of sucrose in taste tests with beverage, yogurt, and other product prototypes

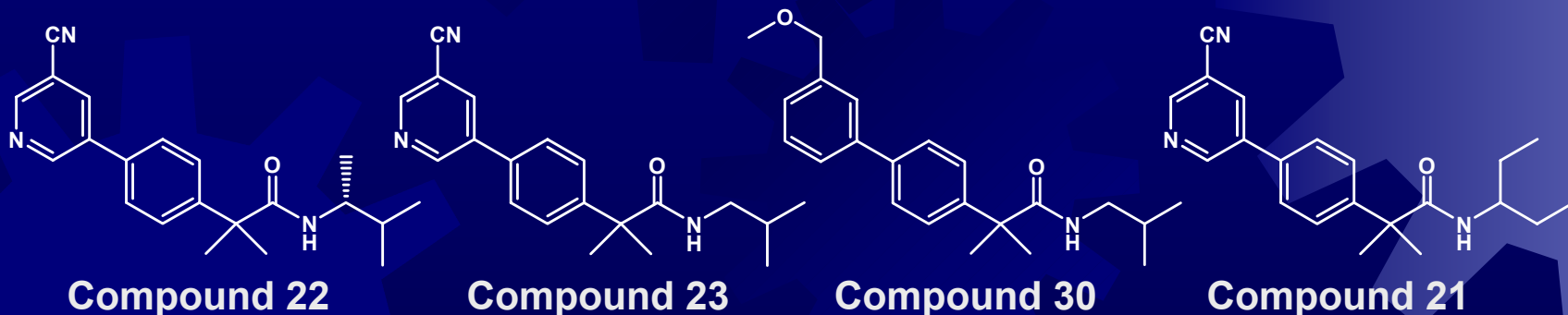
What are **S2383** & **S6973** = ?? At the moment, but...

Synomyx Sweetness Enhancers

% Fructose / Glucose Reduction



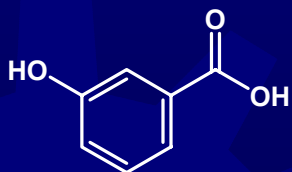
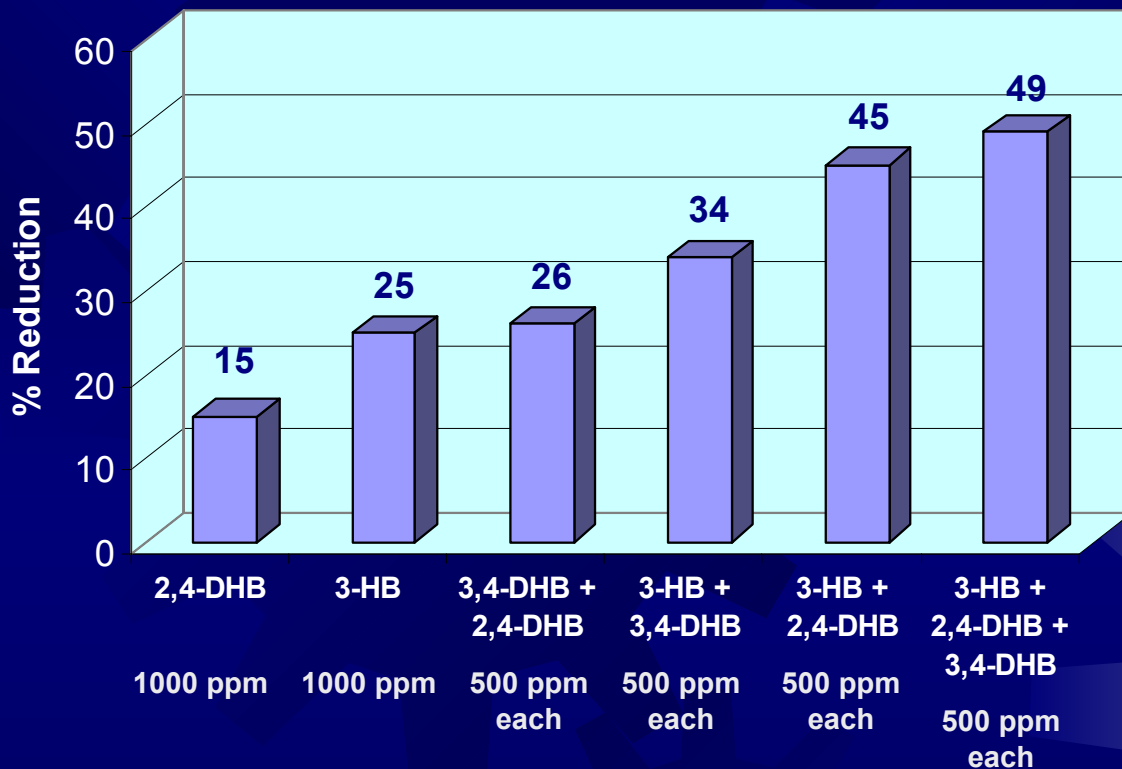
EC_{50} 0.14 μ M EC_{50} 0.15 μ M EC_{50} 0.61 μ M EC_{50} 0.07 μ M



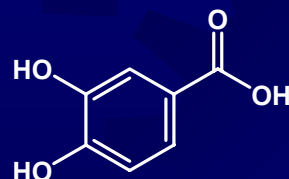
Tachdjian et al.. US Patent Application 20070003680 (2007)

3-Hydroxy & Dihydroxybenzoic acids as Sweetness Enhancers

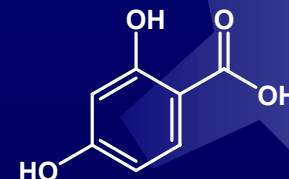
Effect of Blend Ratios on Sucrose Reduction



3-Hydroxybenzoic acid
FEMA 4431



3,4-Dihydroxybenzoic acid
FEMA 4430



2,4-Dihydroxybenzoic acid
FEMA 3798

Bingley et al, US Patent Application 20070054023 (2007) to Cadbury

New GRAS Bitter Blocker

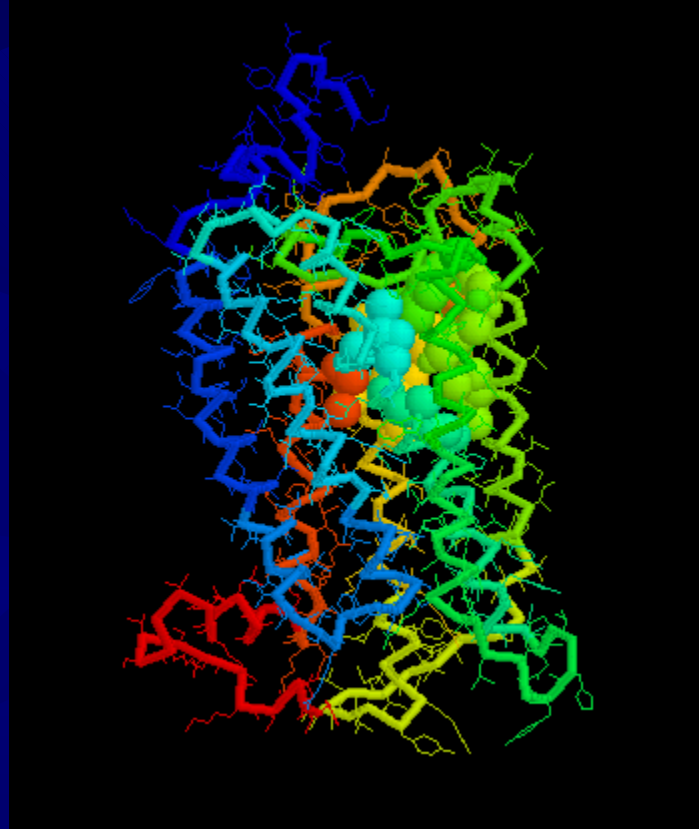


cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid

FEMA 4529

Ungureanu et al., PCT WO2008119197 (Oct. 9, 2008)

Elucidation of Olfactory G-Protein Receptors

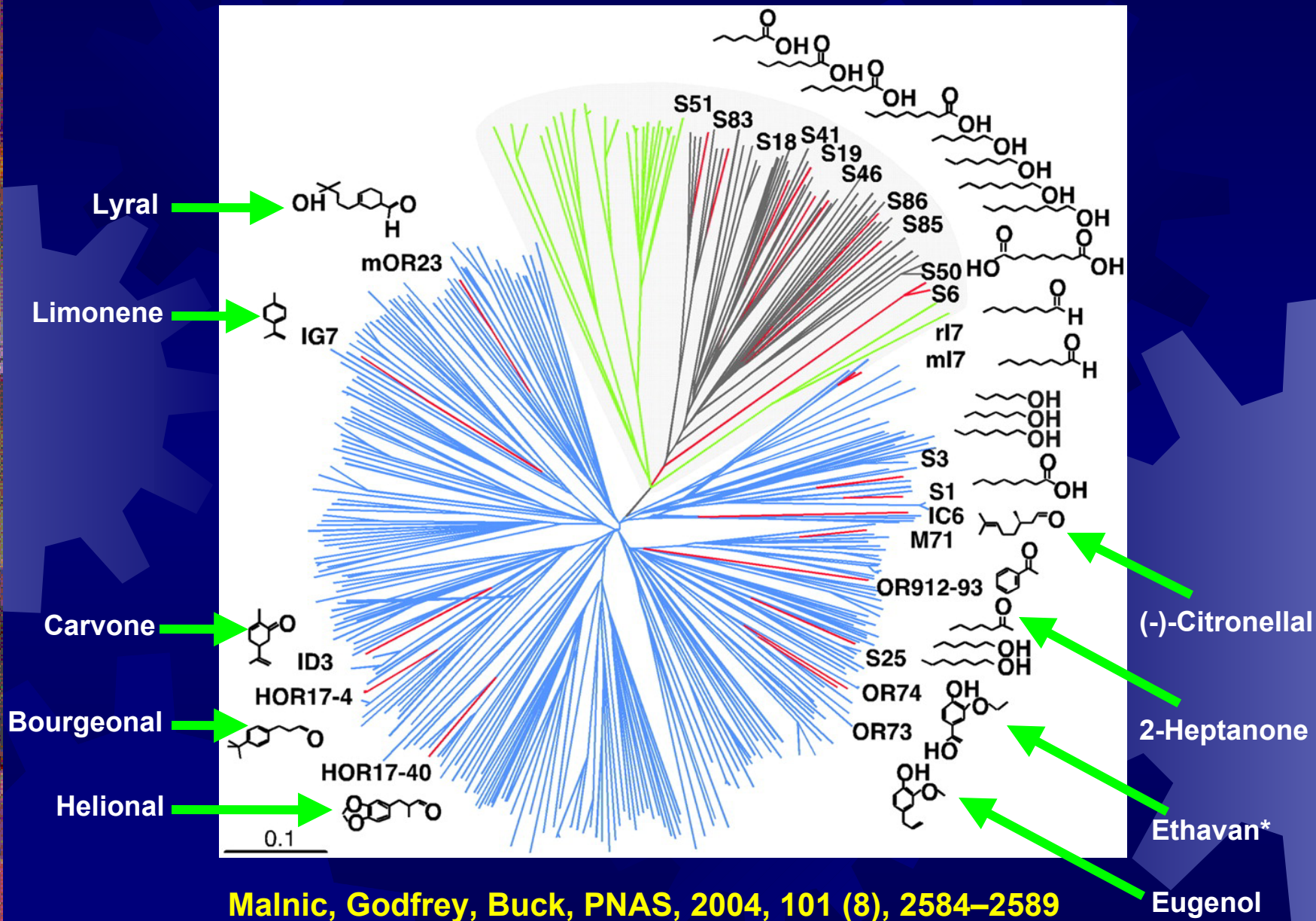


Putative Binding cavity in Human OR1.04.06

900+ Human Olfactory Receptor Genes Identified – D. Lancet
~600 Pseudogenes + ~300 Intact Genes

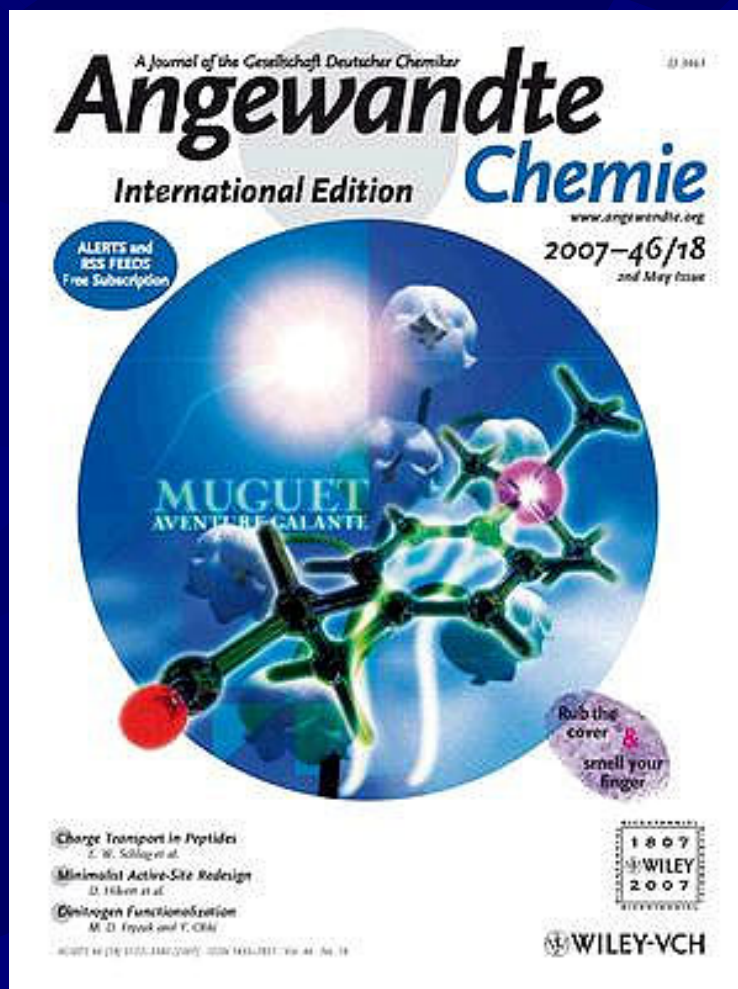
**Glusman, Yanai, Rubin, Lancet, Genome Res. 2001 May;11(5):685-702;
Zozulya, Echeverri, Nguyen, Genome Biology 2001, 2(6):research0018.1–
0018.12; Malnic, Godfrey, Buck, PNAS, 2004, 101 (8), 2584–2589**

Phylogenetic tree of sequence relationships among ORs



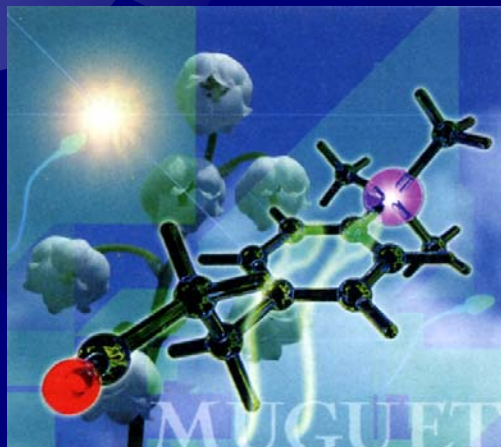
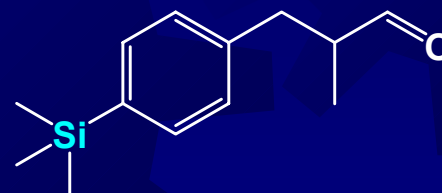
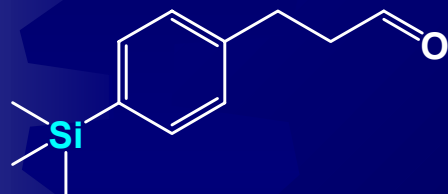
Malnic, Godfrey, Buck, PNAS, 2004, 101 (8), 2584–2589

Prediction of Perception: Probing the hOR17-4 Olfactory Receptor Model with Silicon Analogues of Bourgeonal and Lilial



L. Doszczak, P. Kraft, et al., *Angew. Chemie*, 46 (18), 2007, 3367-3371

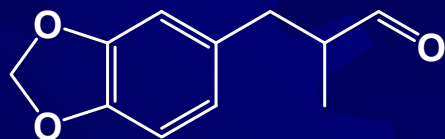
Prediction of Perception: Probing the hOR17-4 Olfactory Receptor Model with Silicon Analogues of Bourgeonal and Lilial



Sense and sensibility: Silicon analogues of the lily-of-the-valley odorants Lilial and Bourgeonal demonstrate that the electronic surface structure determines the interaction of an odorant with its olfactory receptor. The subtle changes in the stereoelectronic properties enable a comparison of in vivo, in vitro, and in silico data. Odor thresholds, as well as the swimming behavior of sperm cells, correlate well with the binding energies obtained from a computational model of the hOR17-4 receptor.

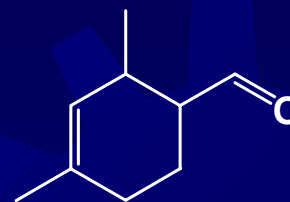
L. Doszczak, P. Kraft, et al., *Angew. Chemie*, 46 (18), 2007, 3367-3371

Fragrance Materials - Newly GRAS



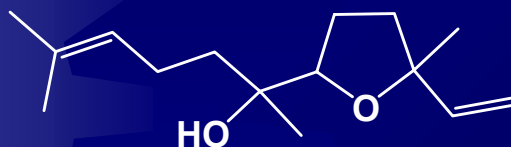
Helional®
FEMA 4599

Floral, green, ozone, marine



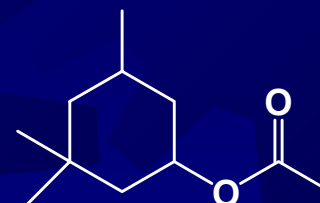
Tripal®, Cyclal C, Vertocitral
FEMA 4505

Green, Citrus, Herbal, Aldehydic



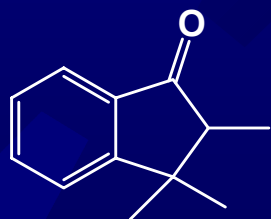
Nerolidol oxide
FEMA 4536

Strawberry- and milk-like fruity
and floral fragrance; red berry flavor



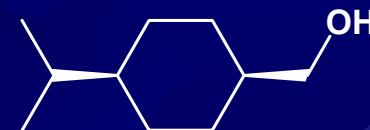
3,3,5-Trimethylcyclohexyl acetate
FEMA 4512

Brightly fresh-fruity, minty,
herb-like and floral-roselike



Safraleine®
FEMA 4556

Leathery, spicy, warm, woody odor,
reminiscent of saffron



Mayol®
FEMA 4507

Fresh floral odor reminiscent of many
flowers - magnolia, tuberose, muguet

The F&F Information Revolution

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Searches any and all ACS journals - (abstracts free)
 - Wiley InterScience -
<http://www3.interscience.wiley.com/search/allsearch>
Searches many journals of F&F interest
 - ScienceDirect - <http://www.sciencedirect.com/>
Searches many journals of F&F interest
- ** In most cases you can purchase individual articles

Industry web sites

- **Perfumer & Flavorist** – <http://www.perfumerflavorist.com/> - great site for industry news; can purchase P&F magazine and J. Essential Oil Res. Articles; Mosciano's database; Bookstore
- **Leffingwell & Associates** – <http://www.leffingwell.com/> - industry news (e.g. Top 10 F&F); lots of technical information & links (all free)
- **JECFA** – <http://www.fao.org/ag/agn/jecfa-flav/search.html> - Search JECFA status and specs
- **Japanese food & flavor additives** - <http://www.ffcr.or.jp/>
- **EU flavor database** – all Flavis numbers
http://ec.europa.eu/food/food/chemicalsafety/flavouring/database/dsp_search.cfm
- **Others** – EFSA, FKS, IOFI, FEMA, Good Scents Co.

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Arctander's Perfume and Flavor Chemicals & Perfume and Flavor Materials of Natural Origin

Originally published by Steffen Arctander in 1969

Perfume and Flavor
Materials of Natural Origin

Perfume and Flavor
Chemicals (Aroma Chemicals)

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- ESO 2006 – Database of Essential Oils
- VCF 2000 – Volatile Compounds in Foods
- PMP 2001 – Database of Perfumery Materials
- FRM 2001 – Database of Flavor Raw Materials
- PFC 2002 – Perfume & Fragrance Classifications

Beverage & Juice Formulation Software

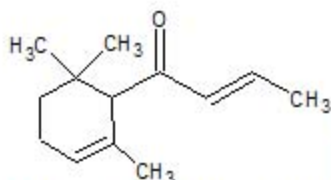
- Beverage-Master 2004
- Juice-Master 2004

Flavor-Base 2007

FLAVOR-BASE PRO "2007"

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Graschem.pics



Molecular formula = C₁₃H₂₀
 Molecular Weight = 192.29
 Composition = C(81.2)
 Molar Refractivity = 59.82
 Molar Volume = 214.0
 Parachor = 492.0
 Index of Refraction = 1.471
 Surface Tension = 27.9 ±
 Density = 0.898
 Polarizability = 23.71

GRAS & EC Chemicals * GRAS & EC Naturals * Your Database * Natural Chemicals * Su...

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GRAS & EC FLAVOR CHEMICALS

Rec. # 500 FEMA No: 3659

Name: Damascone; alpha-Damascone;
 Synonyms: 4-(2,6,6-Trimethyl-2-cyclohexenyl)-2-butene-4-one;
 Suppliers: Firmenich, Moellhausen
 Flavor Description: Fruity (apple-citrus), tea-like with a slight minty note
 Natural Occurrence: Tea.
 Comments: Odor threshold in water: 1.5 ppb for the (+)-alpha-damascone and 100 ppb for the (-)-alpha-damascone (Pickenhagen, 1989). Mosciano, et. al. report that this material has a "sweet, fruity, floral woody with a green berry nuance" odor and a "sweet, fruity, woody with a green seedy background" taste at 30 ppm. alpha-Damascone is very expensive, but does find some utility in Tea, Tobacco and as a modifier in a few Fruit flavors. Except for Tea type applications, the author finds both beta-damascone

COE No. & Cat.: 11053
 FDA No:
 EC Register: 07.134
 JECFA No. 385 Japan: X
 CAS No: 43052-87-5
 Sp. Gravity: 0.898
 Flash Point: >212 F. >100 C.
 EINECS: 256-430-4
 Nature: Nature Identical
 C13 H20 O
 Mol. Wt.: 192.297
 Sol in Water:
 Sol in Ethanol: SOL
 Sol in P.G: SOL
 Sol in Oil: SOL

Image EC Register Japan Flavor Chemicals

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Flavor-Base 2007

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YOUR FLAVOR DATABASE

Record #: 1

FEMA No:

COE No. & Cat.:

[FDA No:](#)

[EC Register:](#)

[JECFA No.](#) Japan:

CAS No:

Sp. Gravity:

Flash Point: F. C.

EINECS:

Nature:

Mol. Wt.:

Sol in Water:

Sol in Ethanol:

Sol in P.G:

Sol in Oil:

Name: "THIS IS YOUR DATABASE"

Synonyms: You may add, edit and delete Records using the buttons below. You may also append records from the graschem.dbf & naturals.dbf files of previous versions of Flavor-Base (See below)

Suppliers:

Flavor Description:

Natural Occurrence: This screen is built on the same format as the GRAS Chemicals screen except that the user can add, edit and delete records.

Comments: This database was designed so that users who had added or edited records to the graschem.dbf or naturals.dbf databases in previous versions of Flavor-Base could easily import (append) records from those prior databases into the database here (yourdata.dbf). This is accomplished by (1.) going into the "Browse" mode, (2.) selecting the "Help" menu at the top of the screen, (3.) selecting Supervisor from the Help menu, (4.) entering you password to access the "Browse Window for

Comments

Image

EC Register

Japan Food Law

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Flavor-Base 2007

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GRAS & EC Chemicals | GRAS & EC Naturals | Your Data | **Natural Chemicals** | Suppliers

SOURCES OF NATURAL FLAVOR CHEMICALS

Rec. #: 1048

FEMA	Natural Chemical	Supplier
3403	Hexenyl hexanoate; cis-3-Hexenyl hexanoate;	Robertet Inc/USA
3403	Hexenyl hexanoate; cis-3-Hexenyl hexanoate;	Buckton Page, Ltd.
3403	Hexenyl hexanoate; cis-3-Hexenyl hexanoate;	Advanced Biotech
3690	Hexenyl lactate; cis-3-Hexenyl lactate;	Fleurchem Inc
3690	Hexenyl lactate; cis-3-Hexenyl lactate;	Penta Manufacturing
3690	Hexenyl lactate; cis-3-Hexenyl lactate;	Robertet Inc/USA

Chemical: **Hexenyl methylbutanoate; 3-Hexenyl 3-methylbutanoate;** FEMA No: 3498

Company: **Robertet Inc/USA** Supplier No: 705

Address: 125 Bauer Drive Contact:

Address: Web: <http://www.robertet.fr/>

City: **Oakland** State: **NJ** Zip: **07436-3190** Comments:

Country: **USA**

Telephone: **201-337-7100** Telex/Fax: **201-337-0070**

Top **Prev** **Next** **Bottom** **Browse** **Query** **Find** **Print Find** **Clear Find** **Add** **Edit** **Delete** **Quit**

Flavor-Base 2007

Bibliography * PPM in Foodstuffs * Natural Occurrence * Odor Threshold Data

Bibliography **PPM In Foodstuffs** Natural Occurrence Odor Thresholds

FOOD NAME **"GRAS" CHEMICALS - PARTS PER MILLION IN FOODSTUFFS**

FOOD NAME	PPM	Name	FEMA
RASPBERRY			
RICE, COOKED	3.5000	Acetaldehyde; Ethanal; Acetic aldehyde;	2003
ROSEMARY	0.0101	Acetoin; 3-Hydroxy-2-butanone; 3-Hydroxybutan-2-one;	2008
RUM	2.1500	Acetone; 2-Propanone; Propan-2-one; Dimethyl ketone	3326
RYE, SOURDOUGH, CRUMBS	0.0299	Acetophenone; Methyl phenyl ketone; Phenyl methyl ketone	2009
SALMON, ATLANTIC, BOILED	0.1250	Amyl alcohol; 1-Pentanol; Pentyl alcohol;	2056
SALMON, ATLANTIC, RAW	0.1049	Benzaldehyde;	2127
SALMON, RAW, SPAWNING	0.0549	Benzyl acetate;	2135
SESAME SEED OIL, DEEP FRY	0.0549	Benzyl alcohol;	2137
SESAME SEED OIL, LIGHT	0.3250	Butanol; 2-Butanol; Butan-2-ol;	
SHALLOT, FRIED	0.0549	Butyl acetate; n-Butyl acetate;	2174
SHRIMP PASTE, FERMENTED	0.0549	Butyl alcohol; Butanol; 1-Butanol; n-Butanol;	2178
SOURSOP	0.0451	Butyl butyrate; Butyl butanoate;	2186
SPEARMINT, NATIVE	0.0049	Butyl hexanoate; Butyl caproate;	2201
SPEARMINT, SCOTCH	0.0049	Butyl isovalerate; n-Butyl 3-methylbutanoate;	2218
SPINY LOBSTER TAIL MEAT	0.0049	Butyl methylbutyrate; n-Butyl 2-methylbutyrate	3393
STRAWBERRY			
SWEET SOP			

Browse All Browse Query Report Find Print Find Clear Find Quit

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Report Designer - flavunit.frx - Page 3 - FLAVOR-BASE PRO "2007"

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Report on:		STRAWBERRY				Page	3
FEMA	COE	FDA	JP	EC REG.	NAME / DESCRIPTION	PPM:	FLAVOR UNIT:
2422	261	172.515	X	09.726	Ethyl benzoate; Threshold in PPB 60.000000 Floral, fruity odor; ylang-ylang like flavor	0.0201	0.33500
2427	264	182.60	X	09.039	Ethyl butyrate; Ethyl butanoate; Threshold in PPB 1.000000 Ethereal, fruity odor; buttery, ripe fruit notes	2.5500	2550.00000
2430	323	172.515	X	09.730	Ethyl cinnamate; Threshold in PPB 17.000000 Sweet, balsamic-cinnamic, honey-like odor and fruity taste	0.0351	2.06470
2432	309	172.515	X	09.059	Ethyl decanoate; Ethyl caprate; Ethyl decylate; Threshold in PPB 44.000000 Sweet, fatty, nut-like, winey-cognac odor	0.0150	0.34090
2439	310	172.515	X	09.060	Ethyl hexanoate; Ethyl caproate; Threshold in PPB 1.000000 Strong, fruity, winey odor; apple, banana, pineapple notes	2.5250	2525.00000
2463	442	172.515	X	09.447	Ethyl isovalerate; Ethyl 3-methylbutanoate; Threshold in PPB 0.400000 Strong, fruity apple odor and taste	0.1549	387.25000
2443	265	172.515	X	09.409	Ethyl methylbutyrate; Ethyl 2-methylbutyrate; Threshold in PPB 0.100000 Strong, green, fruity, apple-strawberry odor and taste	0.5049	5049.00000
2449	392	172.515	X	09.111	Ethyl octanoate; Ethyl caprylate; Ethyl octylate; Threshold in PPB 92.000000 ChemosFruity, winey, sweet odor; cognac-apricot taste	0.1049	1.14021
2456	402	172.515	X	09.121	Ethyl propionate; Ethyl propanoate; Threshold in PPB 9.000000	0.0549	6.10000

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"Legend"

Name of Country

- Permitted in Country
- Banned in Country

Example: Argentina 3,14

The number/s refer to numbered statement/s in the Comment

Press Any Key or Mouse Button to Continue.

Colors * FDA Additives * Code of

Colors

FDA Additives

COLORS

Record #: 5

Name AMARANTH; FD&C RED NO. 2; C.I. ACID RED 27; C.I. FOOD RED 9

Color Index 16185 Color RED EC# E123 FDA#

Argentina	0	2
Australia	0	3
Austria	0	5
Belgium	0	5
Brazil	0	0
Canada	0	3
Chile	0	0
Columbia	0	0
Denmark	0	5
Egypt	X	0
Finland	0	5
France	0	5
Germany	0	5
Greece	0	5
Hong Kong	0	3
India	0	0

Legend for Window

Iran	0	0
Rep. Ireland	0	5
Israel	X	0
Italy	0	5
Japan	0	20
Kuwait	X	0
Luxemburg	0	5
Mexico	0	0
Netherlands	0	5
New Zealand	0	4
Norway	0	5
Pakistan	0	0
Panama	0	0
Peru	0	0

Poland	0	5
Portugal	0	0
Singapore	0	3
South Africa	X	0
Spain	0	5
Sweden	0	5
Switzerland	0	1
Thailand	X	0
Turkey	X	0
United Kingdom	0	5
Uruguay	0	0
United States	X	0
Venezuela	0	0
Yugoslavia	0	0
Zambia	0	0
Zimbabwe	0	0

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Flavor-Base 2007

Colors * FDA Additives * Code of Federal Regulations * USDA Additives * EEC List

Colors **FDA Additives** Title 21 - CFR USDA Additives [EEC List](#)

EUROPEAN COMMUNITY LIST

Name:	Acesulfame K;	Record #:	2
Synonyms:	Acesulfame potassium	EC No:	E950
Function:	Artificial sweetener	COE No:	
Comment:	DIRECTIVE 94/35/EC as amended permits food use as follows: Non-alcoholic drinks — Water-based flavoured drinks, energy-reduced or withno added sugar 350 mg/l — Milk- and milk-derivative-based or fruit-juice-based drinks, energy-reduced or withno added sugar 350 mg/l Desserts and similar products	FEMA No:	
		FDA No:	172.800

[Additives 95/2/EC](#)
[Sweeteners 94/35/EC](#)
[Colours 94/36/EC](#)
[Flavours 88/388/EEC](#)
[Smoke Flavourings](#)

[European Commission "Food Additives" Web Site](#)

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Essential Oils -ESO (update 2006)

The screenshot shows the ESO software interface. The main window is titled "ESO" and has a menu bar with "File", "View", "Sorting", "Report", and "Help". The "Sorting" menu is open, showing options: "Compound by Name", "Compound by Percentage", "Compound by DB1", "Compound by DB5" (checked), and "Compound by CBWX 20M". Below the menu is a list of reference oils, with "Ajowan (Pakistan) seed" selected. The main display area shows a table of compounds and their percentages in the selected sample. The table has columns for "DB 5", "Percentage", and "Compound Name". The "Details" tab is active, showing the name "alpha-Pinene", its synonyms, and its percentage (0.48%) along with minimum and maximum values. The CAS number is also displayed.

DB 5	98.66%	9 compounds in: Ajowan (Pakistan) seed
940.0	0.48	alpha-Pinene
951.6	0.60	Camphene
979.0	1.40	beta-Pinene
1011.6	0.61	delta-3-Carene
1025.7	22.29	para-Cymene
1032.0	1.25	Limonene
1063.7	19.53	gamma-Terpinene
1294.6	46.85	Thymol

Details | **R.I.** | Hide Extra

Name: alpha-Pinene

Synonyms: Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-
2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene

Percentage: 0.48% | Min.: 0.33% | Max.: 0.63%

CAS: 80-56-8

Volatile Compounds in Food – VCF 2000

The screenshot shows the VCF 2000 software interface. The main window is titled "VCF" and has a menu bar with "File", "View", "Report", and "Help". There are two tabs: "Products" and "Compounds". The "Products" tab is active, showing a list of 648 products. "COFFEE" is selected in the list. To the right, the "Compounds" tab is active, showing a list of 834 compounds for "COFFEE". "1-(2-furyl)-1,2-propanedione" is selected in this list. Below the compound list, there is a "Literature" section showing 7 references for the selected compound.

Products List:

- CLODBERRY (*Rubus chamaemorus* L.)
- CLOVE BUD
- CLOVE LEAF
- CLOVE STEM
- CLOVES (*Eugenia caryophyllata* Thunberg)**
- COCOA
- COCOA LIQUOR
- COCONUT (*Cocos nucifera* L.)**
- COCONUT (roasted)
- COCONUT MEAT
- COCONUT MILK
- COCONUT OIL
- COFFEE**
- CORIANDER LEAF (*Coriandrum sativum* L.)
- CORIANDER SEED (*Coriandrum sativum* L.)
- CORN TORTILLAS
- CORN, DENT, OIL
- CORN, SWEET

Compounds List (for COFFEE):

- 2-methylpropanal
- 3-(methylthio)propanal
- 2-oxopropanal
- 2-methylpropane
- 1-(2-furyl)-1,2-propanedione**
- 1-(5-methyl-2-furyl)-1,2-propanedione
- 1-phenylpropane-1,2-dione
- 1-(2-thienyl)-1,2-propanedione
- 1-(3-thienyl)-1,2-propanedione
- propanoic acid

Literature for 1-(2-furyl)-1,2-propanedione:

Reference	Source
+	Helv. Chim. Acta 50 (1967) 628; Stoll et al. (and review) an
+	J. Agric. Food Chem. 16 (1968) 1000; Stoffelsma et al. (an
3.9	Thesis, Berlin (1982); Silwar
+	Z. Lebensm. Unters. Forsch. 184 (1987) 179; Baltes et al.
0.1-15	Chem. Mikrobiol. Technol. Lebensm. 10 (1987) 176; Silwar

The Final Odds & Trends

GC-MS of *Calvatia gigantea* (The Giant Puffball Mushroom)



The giant puffball (*Calvatia gigantea*) is one of the largest of the edible mushroom species. It is usually found in late summer and autumn in meadows, fields, and forests worldwide. It is only edible when fresh and is usually consumed within 24 hours of harvest as the flavor becomes disagreeable on aging.

GC-MS of *Calvatia gigantea* Headspace

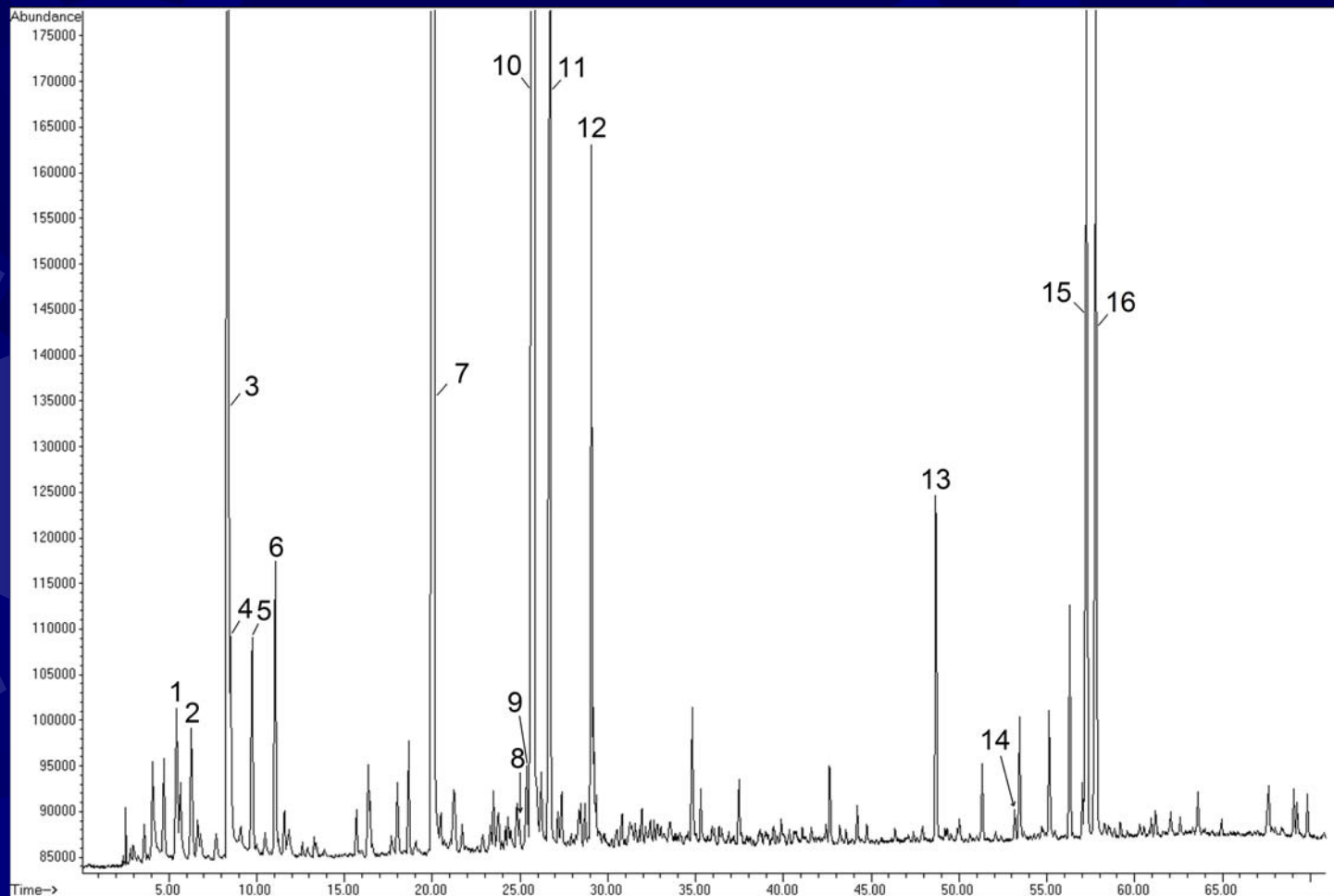
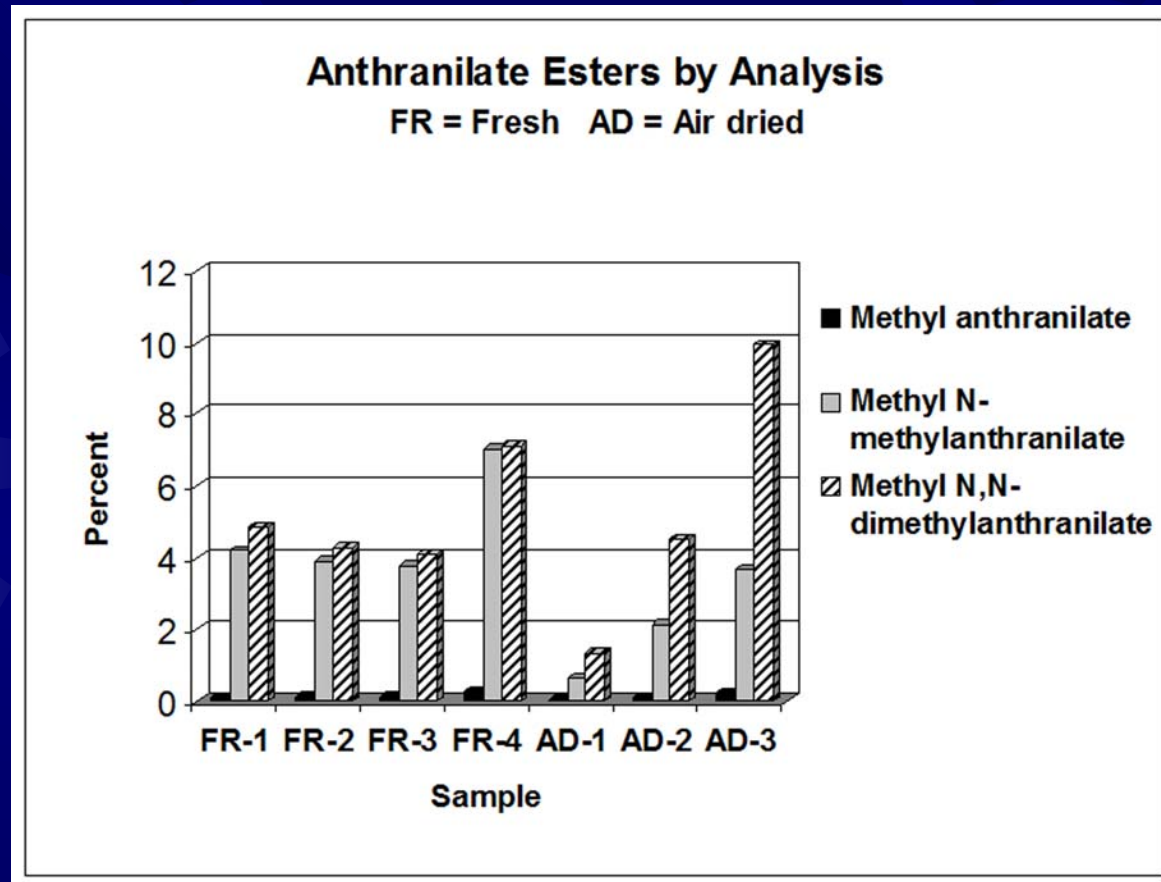


Figure 1. Headspace Chromatogram of Fresh (FR-1) *Calvatia gigantea*
(1) 3-Methylbutanal (2) 2-Pentanone (3) Isoamyl alcohol (4) 2-Methyl-1-butanol (5) Toluene (6) 1-Octene (7) Anisole (8) 1-Octen-3-one (9) 1-Octen-3-ol (10) 3-Octanone (11) 3-Octanol (12) Limonene (13) N-(2-methylphenyl)formamide^{tent} (14) Methyl anthranilate (15) Methyl N,N-dimethylantranilate (16) Methyl N-methylantranilate

GC-MS of *Calvatia gigantea* Headspace



Significance – First isolation of anthranilates from a mushroom species

Source: Leffingwell & Alford, manuscript in preparation