Sensory profile analysis: Preliminary characterization of wine aroma profiles using solid phase microextraction and simultaneous chemical and sensory analyses

Iowa State University and South Dakota State University
Ames, IA

Somchai Rice, Jacek Koziel*, Devin Maurer*, Anne Fennell***
**Department of Agricultural and Biosystems Engineering, Iowa State University*
***Department of Plant Science, South Dakota State University*

Background and Rationale: *Sensory profile analysis* (iv) is part of *Obj. 1a Evaluate cold climate cultivar performance under a wide range of climates throughout the Upper Midwest and Northeast to match cultivar with site*. Wine aroma profiles from three wine varieties (Marquette, Frontenac, and St. Croix, 2012 SDSU) were characterized. Results will be compared with the development of volatiles in crushed berries, and volatiles emitted by maturing grapes to inform how grape growing and processing can affect wine aroma.

Treatments/Methods:
Wine aroma profiles from a selection of the sites will be characterized using solid phase microextraction coupled with multidimensional gas chromatography-mass spectrometry-olfactometry for simultaneously chemical and sensory analysis. This method couples identification of flavor and aroma-active compounds with detection and description by humans. Preliminary work has been completed with 2012 Marquette, Frontenac, and St. Croix wine in anticipation of the major effort with wine aroma analyses in years 2 to 4.

An aromagram was recorded by a panelist utilizing the human trained panelist using nose as a detector. Aroma events resulting from separated compounds eluting from the gas chromatography column were characterized for aroma descriptor with a 64-descriptor panel and aroma intensity with Aromatrax software (MOCON Texas Laboratory, Round rock, TX). The olfactory responses of a panelist were recorded using AromaTrax software by applying an aroma tag to a peak or a region of the chromatographic separation.

Results:

Examples of simultaneous chemical and sensory analyses of Marquette, Frontenac, and St. Croix wine are presented in the following figures and tables.

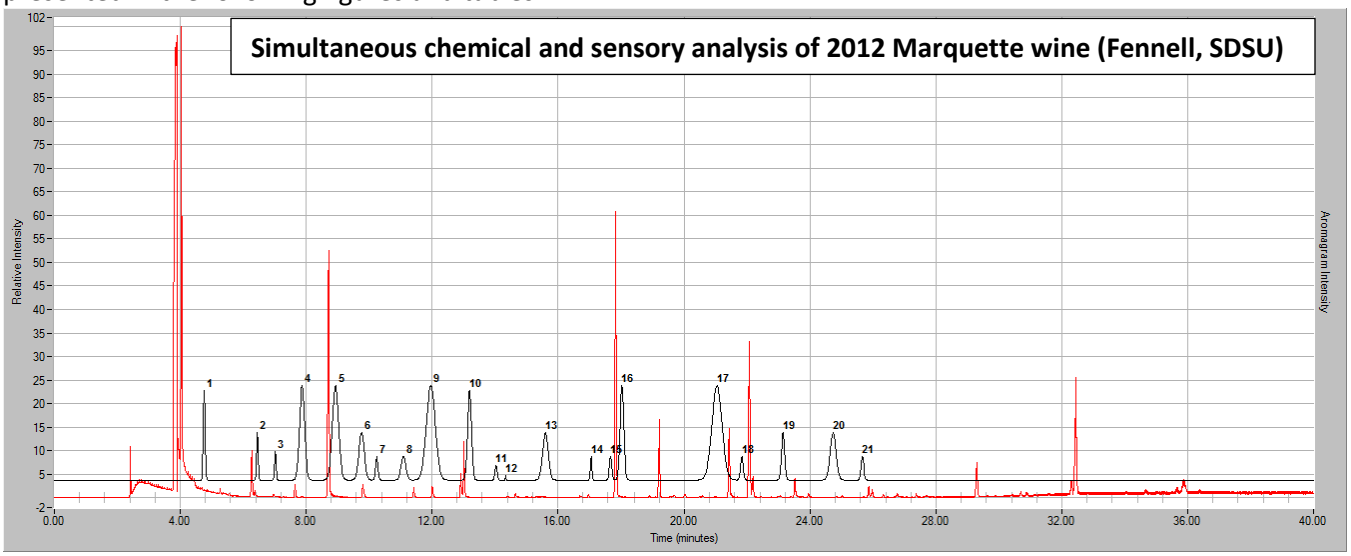

Figure 1|Example of a typical overlay of total ion chromatogram (TIC) and aromagram showing simultaneous chemical and sensory analysis of Marquette wine using multidimensional gas chromatography-mass spectrometry-olfactometry. Red signal is TIC from mass selective detector, black signal is aromagram generated by trained human panelist. Details for each signal are given in Table 1.

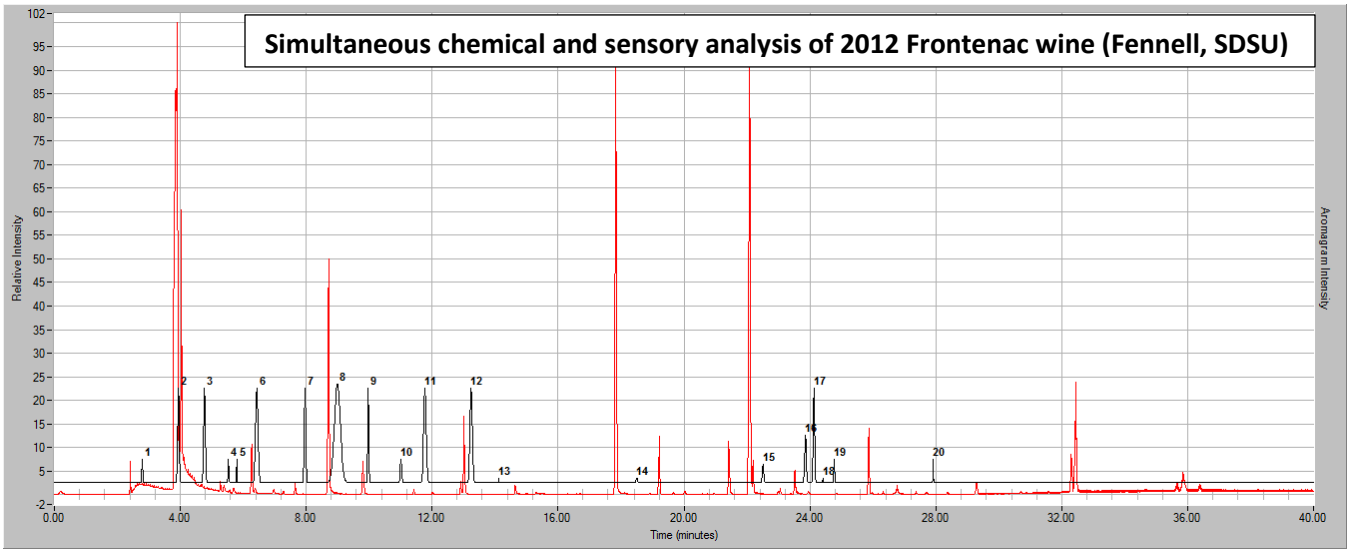

Figure 2|Example of a typical overlay of total ion chromatogram (TIC) and aromagram showing simultaneous chemical and sensory analysis of Frontenac wine using multidimensional gas chromatography-mass spectrometry-olfactometry. Red signal is TIC from mass selective detector, black signal is aromagram generated by trained human panelist. Details for each signal are given in Table 2.

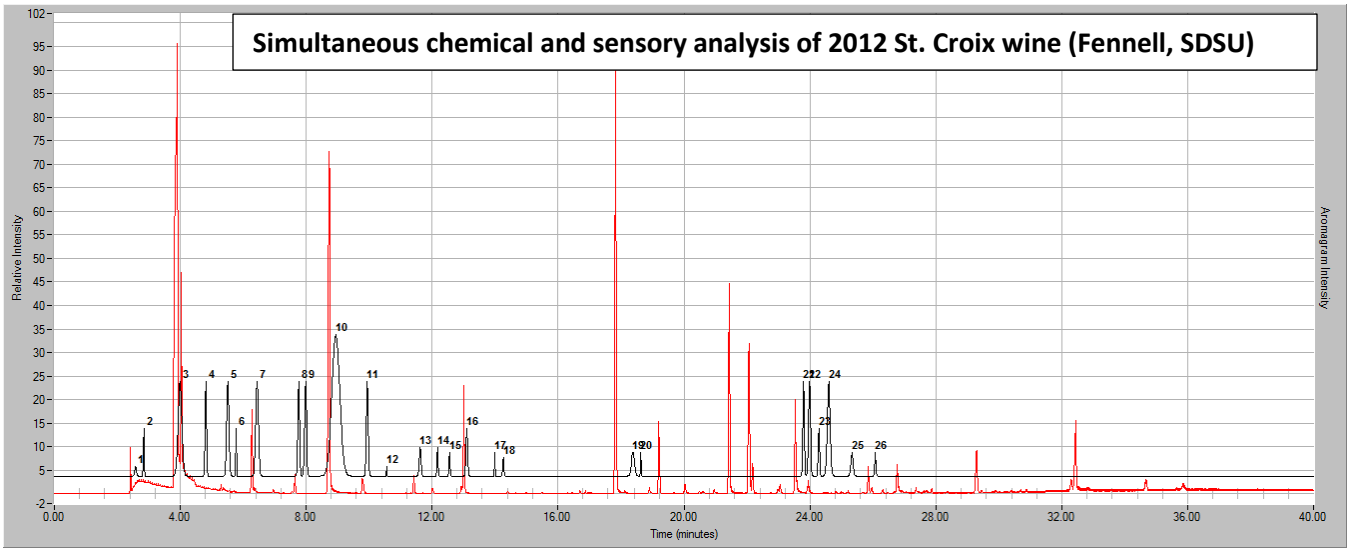

Figure 3|Example of a typical overlay of total ion chromatogram (TIC) and aromagram showing simultaneous chemical and sensory analysis of St. Croix wine using multidimensional gas chromatography-mass spectrometry-olfactometry. Red signal is TIC from mass selective detector, black signal is aromagram generated by trained human panelist. Details for each signal are given in Table 3.

What the results mean:

- Preliminary simultaneous chemical and sensory analysis of Marquette, Frontenac, and St. Coix wine shows 60+ chemical compounds of which more than 20+ produce distinct flavor aroma as detected by human nose.
- Many of the aromas are desirable for enhanced wine aroma.
- There is no data comparing cold climate wine aromas with wines currently marketed.
- Comparisons and benchmarking of aromas in wines made from cold hardy grapes is warranted.

Table 1| Summary of compounds detected using simultaneous chemical and sensory analysis of Marquette wine.

Peak #	RT(min)	Compound	CAS	% Match	Published Aroma Descriptor[1]	Detected Aroma Descriptor
	3.32	Methyl acetate	79-20-9	82		
	3.95	Propylene glycol	57-55-6	68		
	4.04	n-Propyl acetate	109-60-4	70	Fruit, Apple, Banana	
1	4.68					Butter
	5.32	3-pentanol	584-02-1	73	Fruit	
	6.37	Ethyl isobutyrate	97-62-1	90	Sweet, Rubber	
	6.38	Propyl butyrate	105-66-8	73	Pineapple, Solvent	
2	6.39					Fruity
3	6.96					Neutral
	6.97	Isobutyl acetate	110-19-0	79		
	7.28	1-butanol	71-36-3	84	Medicine, Fruit	
	7.64	Ethyl butyrate	105-54-4	96	Apple	
4	7.66					Neutral 0/ Fruity
5	8.66					Unpleasant -1/Skunk/Fruity
	8.71	Amyl alcohol	71-41-0	96	Balsamic	
	8.72	3-methylpentane	96-14-0	75		
	8.97	Ethyl 3-methylbutanoate	108-64-5	74	Fruit	
6	9.52					Neutral 0/ Cut Grass/ Floral
	9.80	Isoamyl acetate	123-92-2	96	Banana	
	9.80	Amyl acetate	628-63-7	90		
7	10.14					Neutral 0/ Cut Grass
8	10.88					Neutral 0/ Cut Grass
	11.41	Ethyl lactate	97-64-3	97	Fruit	
9	11.57					Neutral 0
	12.00	1-Hexanol	111-27-3	96	Resin, Flower, Green	
	12.89	Acetic acid	64-19-7	100	Sour	
	13.02	Ethyl hexanoate	123-66-0	95	Apple peel, Fruit	
10	13.03					Floral/Skunk
11	13.95					Pleasant +2
12	14.32					Neutral 0
	14.39	1-Heptanol	111-70-6	87	Chemical, Green	
	14.40	Methacrolein	78-85-3	68		
	15.16	Isobutyric acid	79-31-2	66	Rancid, Butter, Cheese	
13	15.36					Neutral 0/ Burnt match
	15.50	Ethyl heptanoate	106-30-9	72	Fruit	
	16.58	γ-butyrolactone	96-48-0	77	Caramel, Sweet	
	16.71	1-Octanol	111-87-5	88	Chemical, Metal, Burnt	

	16.97	Linalool	78-70-6	82	Flower, Lavender	
14	16.98					Pleasant +1/ Floral
15	17.57					Unpleasant -3/ Unpleasant -2
	17.83	Ethyl octanoate	106-32-1	100	Fruit, Fat	
16	17.87					Pleasant +3/ Floral
	18.89	Cyclohexane	110-82-7	67		
	18.91	1-Nonanol	143-08-8	84	Fat, Green	
	18.91	5-octanolide	698-76-0	66	Peach	
	19.56	Isopentyl acetate	29460-92-2	73		
	19.56	(+)-4-Carene	29050-33-7	74		
	19.71	α-terpineol	98-55-5	74	Oil, Anise, Mint	
	20.02	Ethyl nonanoate	123-29-5	82		
	20.04	Heptanoic acid	111-14-8	85		
	20.04	Pentanoic acid	109-52-4	85	Sweat	
	20.49	Citronellol	106-22-9	81	Rose	
	20.59	Methyl salicylate	119-36-8	95	Peppermint	
17	20.62					Neutral 0/ Smokey/ Rubber
	20.64	Benzyl alcohol	100-51-6	77		
	21.43	Phenylethyl alcohol	60-12-8	99	Honey, Spice, Rose, Lilac	
	21.48	Phenethyl isobutyrate	103-48-0	79		
	21.71	Ethyl salicylate	118-61-6	83	Wintergreen, Mint	
18	21.72					Neutral 0/ Burnt Match
	22.08	Ethyl decanoate	110-38-3	99	Grape	
	22.99	2,3,4-trimethylpentane	565-75-3	66		
	23.00	Isoamyl octanoate	2035-99-6	81		
19	23.01					Floral
	23.07	β-damascenone	23726-93-4	87	Apple, Rose, Honey	
	23.52	Octanoic Acid	124-07-2	94	Sweat, Cheese	
20	24.49					Neutral 0/ Berry
	24.85	Octyl formate	112-32-3	71		
	25.03	Butylated Hydroxytoluene	128-37-0	86		
21	25.56					Neutral 0/ Berry
	25.69	Eugenol	97-53-0	79	Clove, Honey	
	25.87	Ethyl laurate	106-33-2	93	Leaf	
	26.33	Nerolidol	7212-44-4	69	Wood, Flower, Wax	
	26.49	Ethylhydroxyhexanoate	2305-25-1	66	Fresh	
	26.76	n-Decanoic acid	334-48-5	80	Rancid, Fat	
	27.88	β-irone	79-70-9	71		
	29.31	Ethyl tetradecanoate	124-06-1	94	Ether	
	30.89	Ethyl undecanoate	627-90-7	70	Cognac, Coconut	
	31.59	1-undecanol	112-42-5	75	Mandarin	

	32.45	Ethyl hexadecanoate	628-97-7	97	Wax
	35.86	Methyl linoleate	112-63-0	68	
	35.92	Ethyl stearate	111-61-5	71	
	36.38	Camphene	79-92-5	65	Camphor

Peak # corresponds to numbered peaks in aromagram (black signal) of Figure 1. RT = retention time in minutes. % Match = net probability match of mass spectra of sample to target specialty mass spectral library. Published Aroma Descriptor compiled from Flavornet[1]. Detected Aroma Descriptor is generated by trained human panelist.

Table 2| Summary of compounds detected using simultaneous chemical and sensory analysis of Frontenac wine.

Peak #	RT(min)	Compound	CAS	% Match	Published Aroma Descriptor[1]	Detected Aroma Descriptor
	2.67	Acetaldehyde	75-07-0	71	Pungent, Ether	
1	2.76					Unpleasant -1
2	3.87					Ethanol
	3.91	Propylene glycol	57-55-6	68		
	4.03	n-Propyl acetate	109-60-4	70	Fruit, Apple, Banana	
	4.68	2-Pentanone	107-87-9	80	Ether, Fruit	
3	4.70					Butter
	5.28	3-pentanol	584-02-1	75	Fruit	
4	5.50					Floral
	5.56	Propyl propanoate	106-36-5	66	Pineapple	
5	5.76					Neutral
	6.26	Methyl acetate	79-20-9	72		
6	6.33					Sweaty/Floral
	6.38	2-methyl-3-pentanone	565-69-5	84	Mint	
	6.96	Butyl acetate	123-86-4	91	Pear	
	6.98	Isobutyl acetate	110-19-0	89	Fruit, Apple, Banana	
	7.27	1-butanol	71-36-3	94	Medicine, Fruit	
	7.65	Ethyl butyrate	105-54-4	96	Apple	
7	7.90					Pleasant +1/ Sherry
	8.71	Amyl alcohol	71-41-0	96	Balsamic	
8	8.73					Sweaty/Floral/Strawberry
	8.74	3-methylpentane	96-14-0	79		
	8.96	Methyl propionate	554-12-1	67		
	8.97	Ethyl 3-methylbutanoate	108-64-5	72	Fruit	
	9.80	Isoamyl acetate	123-92-2	97	Banana	
9	9.93					Banana
10	10.95					Medicinal
	11.41	Ethyl lactate	97-64-3	95	Fruit	
11	11.66					Taco Shell
	12.01	1-hexanol	111-27-3	87	Resin, Flower, Green	

	12.91	Acetic acid	64-19-7	100	Sour	
	13.02	Ethyl hexanoate	123-66-0	98	Apple peel, Fruit	
12	13.15					Cherry/Fruity
13	14.12					Garlic
	14.41	1-Heptanol	111-70-6	79	Chemical, Green	
	14.64	5-methyl-3-heptanone	541-85-5	70		
	15.50	Ethyl heptanoate	106-30-9	71	Fruit	
	16.29	2-methylvaleric acid	97-61-0	68		
	16.30	Methylbutyric acid	116-53-0	71	Cheese, Sweat	
	16.58	γ-butyrolactone	96-48-0	80	Caramel, Sweet	
	16.70	1-Octanol	111-87-5	81	Chemical, Metal, Burnt	
	17.84	Ethyl octanoate	106-32-1	100	Fruit, Fat	
14	18.44					Unpleasant -1
	18.91	2-ethyl-1-butanol	97-95-0	69		
	18.92	5-octanolide	698-76-0	71	Peach	
	19.90	Propyl octanoate	624-13-5	67		
	20.01	2-ethyl butyric acid	88-09-5	78		
	20.02	Ethyl nonanoate	123-29-5	81		
	20.03	Heptanoic acid	111-14-8	86		
	20.03	Pentanoic acid	109-52-4	87	Sweat	
	20.59	Methyl salicylate	119-36-8	93	Peppermint	
	20.76	Methyl decanoate	110-42-9	66	Wine	
	20.77	Hexanoic acid, methyl ester	106-70-7	68	Fruit, Fresh, Sweet	
	20.97	Octyl formate	112-32-3	84		
	21.43	Phenylethyl alcohol	60-12-8	99	Honey, Spice, Rose, Lilac	
	21.48	Phenethyl isobutyrate	103-48-0	69		
	22.09	Ethyl decanoate	110-38-3	96	Grape	
15	22.45					Fruity
	22.51	2-methyl naphthalene	91-57-6	78		
	23.00	Isoamyl octanoate	2035-99-6	83		
	23.06	β-damascenone	23726-93-4	94	Apple, Rose, Honey	
	23.52	Octanoic Acid	124-07-2	98	Sweat, Cheese	
16	23.79					Spicy
17	24.08					Raspberry
18	24.39					Strawberry
19	24.74					Strawberry Jam
	24.85	1-Nonanol	143-08-8	72	Fat, Green	
	25.87	Ethyl laurate	106-33-2	96	Leaf	
	26.20	γ-hexalactone	695-06-7	67	Coumarin, Sweet	
	26.33	Nerolidol	7212-44-4	79	Wood, Flower, Wax	
	26.72	2,3,4-trimethylpentane	565-75-3	75		

	26.76	n-Decanoic acid	334-48-5	93	Rancid, Fat	
20	27.89					Fruity
	28.38	1-undecanol	112-42-5	86	Mandarin	
	29.30	Ethyl tetradecanoate	124-06-1	93	Ether	
	31.58	1-Decanol	112-30-1	66	Fat	
	32.44	Ethyl hexadecanoate	628-97-7	98	Wax	
	35.66	Methyl oleate	112-62-9	71		
	35.86	Methyl linoleate	112-63-0	72		
	35.91	Ethyl stearate	111-61-5	67		
	36.38	Perillaldehyde	2111-75-3	67	Spice	
	36.39	(1R)-(+)-trans-isolimonene	5113-87-1	65		
	36.39	Camphene	79-92-5	66	Camphor	
	36.40	Caryophyllene oxide	1139-30-6	66	Herb, Sweet, Spice	

Peak # corresponds to numbered peaks in aromagram (black signal) of Figure 2. RT = retention time in minutes. % Match = net probability match of mass spectra of sample to target specialty mass spectral library. Published Aroma Descriptor compiled from Flavornet[1]. Detected Aroma Descriptor is generated by trained human panelist.

Table 3| Summary of compounds detected using simultaneous chemical and sensory analysis of St. Croix wine.

Peak #	RT(min)	Compound	CAS	% Match	Published Aroma Descriptor[1]	Detected Aroma Descriptor
1	2.52					Sweet
	2.67	Acetaldehyde	75-07-0	88	Pungent, Ether	
2	2.80					Unpleasant -1
	3.31	Methyl acetate	79-20-9	76		
3	3.83					Alcoholic/Sweet
	4.03	n-Propyl acetate	109-60-4	70	Fruit, Apple, Banana	
4	4.75					Buttery
	5.36	3-pentanol	584-02-1	70	Fruit	
5	5.42					Fruity
6	5.74					Body Odor
7	6.33					Pleasant +1/Unpleasant -1/Fruity
	6.38	Ethyl isobutyrate	97-62-1	87	Sweet, Rubber	
	6.97	Isobutyl acetate	110-19-0	89	Fruit, Apple, Banana	
	6.98	Butyl acetate	123-86-4	73	Pear	
	7.29	1-butanol	71-36-3	90	Medicine, Fruit	
	7.64	Ethyl butyrate	105-54-4	98	Apple	
8	7.70					Strawberry
9	7.90					Spicy
10	8.60					Body Odor/Woody/Body Odor/Chocolate/Cherry

	8.75	Amyl alcohol	71-41-0	94	Balsamic	
	8.75	3-methylpentane	96-14-0	81		
	8.96	Ethyl 3-methylbutanoate	108-64-5	83	Fruit	
	8.98	2,2-Dimethylvaleric acid	1185-39-3	65		
	9.57	Ethyl (E)-2-crotonate	623-70-1	73		
	9.81	Isoamyl acetate	123-92-2	98	Banana	
11	9.87					Strawberry Jam
12	10.53					Sweet
	11.42	Ethyl lactate	97-64-3	94	Fruit	
13	11.55					Unpleasant -1/Medicinal
	12.01	1-hexanol	111-27-3	93	Resin, Flower, Green	
14	12.13					Fruity
15	12.51					Nutty
	12.92	Acetic acid	64-19-7	100	Sour	
	12.93	Methyl formate	107-31-3	81		
	13.01	Ethyl hexanoate	123-66-0	98	Apple peel, Fruit	
16	13.04					Floral/Fruity
17	13.97					Spicy
18	14.21					Taco Shell
	14.40	1-Heptanol	111-70-6	94	Chemical, Green	
	14.40	Butyl formate	592-84-7	68		
	14.66	Propylene glycol	57-55-6	76		
	15.00	Ethyl 3-hydroxybutanoate	5405-41-4	67	Marshmallow	
	15.18	Isobutyric acid	79-31-2	70	Rancid, Butter, Cheese	
	15.48	Ethyl heptanoate	106-30-9	83	Fruit	
	16.29	Methyl octanoate	111-11-5	69	Orange	
	16.70	1-Octanol	111-87-5	93	Chemical, Metal, Burnt	
	16.87	2,3,4-trimethylpentane	565-75-3	74		
	16.97	Linalool	78-70-6	68	Flower, Lavender	
	17.03	Isovaleric acid	503-74-2	78	Sweat, Acid, Rancid	
	17.05	Methylbutyric acid	116-53-0	81	Cheese, Sweat	
	17.83	Ethyl octanoate	106-32-1	100	Fruit, Fat	
19	18.25					Rusty/Metallic/Medicinal
20	18.61					Woody
	18.89	1-Nonanol	143-08-8	92	Fat, Green	
	20.01	Ethyl nonanoate	123-29-5	68		
	20.04	Pentanoic acid	109-52-4	78	Sweat	
	20.49	Citronellol	106-22-9	88	Rose	
	20.50	Citronellyl butyrate	141-16-2	88	Fruit, Sweet, Rose	
	20.50	Citronellolformate	105-85-1	66		
	20.59	Methyl salicylate	119-36-8	94	Peppermint	

	20.65	Benzyl alcohol	100-51-6	90	Sweet, Flower	
	20.96	Octyl formate	112-32-3	67		
	20.97	Dimethyl octanol	106-21-8	78		
	21.05	Ethyl phenylacetate	101-97-3	66	Fruit, Sweet	
	21.44	Phenylethyl alcohol	60-12-8	99	Honey, Spice, Rose, Lilac	
	21.47	Phenethyl isobutyrate	103-48-0	71		
	21.51	Geraniol	106-24-1	66	Rose, Geranium	
	22.07	Ethyl decanoate	110-38-3	99	Grape	
	22.99	Isoamyl octanoate	2035-99-6	87		
	23.05	β-damascenone	23726-93-4	96	Apple, Rose, Honey	
	23.54	Octanoic Acid	124-07-2	95	Sweat, Cheese	
21	23.74					Sweet
22	23.91					Sweet/Floral
23	24.24					Honey/Pear
24	24.48					Sweet/Strawberry
	24.69	Phenethyl isovalerate	140-26-1	70		
	24.72	Phenethyl phenyl acetate	102-20-5	73		
	24.85	1-undecanol	112-42-5	83	Mandarin	
	25.02	Butylated Hydroxytoluene	128-37-0	80		
25	25.25					Fruity
	25.69	Eugenol	97-53-0	67	Clove, Honey	
	25.87	Ethyl laurate	106-33-2	94	Leaf	
26	26.03					Woody
	26.20	γ-hexalactone	695-06-7	66	Coumarin, Sweet	
	26.32	Ethyl cinnamate	103-36-6	78	Honey, Cinnamon	
	26.33	Nerolidol	7212-44-4	73	Wood, Flower, Wax	
	26.47	Ethylhydroxyhexanoate	2305-25-1	69	Fresh	
	26.78	n-Decanoic acid	334-48-5	96	Rancid, Fat	
	29.29	Ethyl tetradecanoate	124-06-1	96	Ether	
	29.90	(-)-β-Citronellene	10281-56-8	68		
	30.89	Ethyl undecanoate	627-90-7	65	Cognac, Coconut	
	32.43	Ethyl hexadecanoate	628-97-7	97	Wax	
	35.85	Methyl linoleate	112-63-0	70		
	35.89	Ethyl stearate	111-61-5	76		

Peak # corresponds to numbered peaks in aromagram (black signal) of Figure 3. RT = retention time in minutes. % Match = net probability match of mass spectra of sample to target specialty mass spectral library. Published Aroma Descriptor compiled from Flavornet[1]. Detected Aroma Descriptor is generated by trained human panelist.

References

[1]Acree, T., and H. Arn. 2004. Flavornet. Available at http://www.flavornet.org/flavornet.html (verified 03 Jan 2014).