

## **A comprehensive overview of common e-liquid ingredients and how they can be used to predict an e-liquid's flavor category**

Erna JZ Krüsemann<sup>1,2\*</sup>, Anne Havermans<sup>1\*</sup>, Jeroen LA Pennings<sup>1</sup>, Kees de Graaf<sup>2</sup>, Sanne Boesveldt<sup>2</sup>, Reinskje Talhout<sup>1</sup>

*\* These authors contributed equally*

<sup>1</sup> Centre for Health Protection, National Institute for Public Health and the Environment (RIVM), Antonie van Leeuwenhoeklaan 9, 3721 MA Bilthoven, The Netherlands

<sup>2</sup> Division of Human Nutrition and Health, Wageningen University, Stippeneng 4, 6708 WE Wageningen, The Netherlands

Corresponding author: Erna JZ Krüsemann, Centre for Health Protection, National Institute for Public Health and the Environment (RIVM), Antonie van Leeuwenhoeklaan 9, 3721 MA Bilthoven, The Netherlands, [erna.krusemann@rivm.nl](mailto:erna.krusemann@rivm.nl), +31 302742512

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**Supplementary Table S1**

**Table S1:** An overview of all 219 unique ingredients reported to be added to at least 100 e-liquids of the entire data set, including the percentage of e-liquids containing the ingredient. This overview covers 99.4% of all ingredients reported. The non-flavoring ingredients (n=6) are marked in grey and highlighted with an asterisk (\*).

<b>E-liquid ingredient</b>	<b>E-liquids containing the ingredient (% of total number of e-liquids)</b>
2,3-Pentanedione	3.09%
1-Pentanol	1.05%
1,4-Dimethoxybenzene	1.91%
2-3-Hexanedione	1.07%
2-Acetyl Furan	1.18%
2-Acetyl Pyridine	1.96%
2-Acetylpyrazine	6.00%
2-Ethyl-3-methyl pyrazine	0.79%
2-Isopropyl-4-methyl thiazole	0.47%
2-Isopropyl-N,2,3-trimethylbutyramide	1.28%
2-Methoxy-3-methyl pyrazine	0.47%
2-Methyl Butyric Acid	9.77%
2-Methylbutyl acetate	2.23%
2-Phenylethanol	4.20%
2-Phenylethyl Acetate	0.57%
2-Propanol	1.43%
2,3-Dimethylpyrazine	2.08%
2,3,5-Trimethylpyrazine	5.67%
2,3,5,6-Tetramethylpyrazine	2.90%
2,5-Dimethylpyrazine	1.54%
2,6-Dimethyl-5-heptenal	2.15%
4-(4-Hydroxyphenyl)-2-butanone	9.43%
4-(4-methoxyphenyl)butan-2-one	1.06%
4-Methyl-5-Thiazole Ethanol	5.53%
4-Terpinenol	0.37%
4,5-Dimethyl-3-Hydroxy-2,5-Dihydrofuran-2-One	1.38%
5-methyl-2-Phenyl-2-Hexenal	1.10%
5-Methyl Furfural	2.73%
6-Methyl-5-Hepten-2-one	0.80%
6-Methyl Coumarin	0.60%
Acetal	1.08%
Acetaldehyde	2.02%
Acetic Acid	15.67%
Acetoin	7.47%
Allyl Hexanoate	5.54%
alpha-Damascenone	0.02%
alpha-Damascone	1.84%
Alpha-Ionone	5.55%
alpha-Methylbenzyl acetate	1.80%
alpha-Pinene	2.14%
alpha-Terpineol	5.51%

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Amyl acetate	1.88%
Amyl Butyrate	1.10%
Anethole	2.30%
Anisaldehyde	9.01%
Anise Oil	0.97%
Anisyl Acetate	0.83%
Anisyl Alcohol	7.04%
Benzaldehyde	12.43%
Benzaldehyde propylene glycol acetal	0.74%
Benzyl Acetate	9.20%
Benzyl Alcohol	14.19%
Benzyl Benzoate	3.10%
Benzyl Butyrate	1.41%
beta-Caryophyllene	1.81%
beta-Damascenone	4.42%
beta-Damascone	5.53%
Beta-Ionone	7.54%
beta-Pinene	2.14%
Blood Orange Oil	1.48%
Bucchu Leaf Oil	1.28%
Butyl Acetate	2.33%
Butyl Butyrate	2.82%
Butyl Butyryl Lactate	3.95%
Butyric Acid	14.99%
Capsicum oleoresin	0.48%
Caramel	2.38%
Carob	1.47%
Carvone	1.45%
Cassia oil	1.25%
Cedrol	2.08%
Cinnamaldehyde	3.78%
Cinnamon Oil	0.99%
Cinnamyl alcohol	0.82%
Cis-3-hexenol	17.77%
Cis-3-hexenyl Acetate	9.18%
Cis-3-Hexenyl Butyrate	3.35%
Cis-3-Hexenyl Isovalerate	0.78%
cis-6-Nonen-1-ol	0.93%
Citral	5.62%
Citric Acid	3.10%
Citronellol	1.88%
Citronellyl Acetate	1.50%
Cocoa Extract	1.54%
Coffee Extract	0.34%
Cornmint Oil	1.26%
D-Carvone	0.35%
Decanal	1.25%
Decanoic Acid	1.94%
delta-Decalactone	11.21%
delta-Dodecalactone	8.65%

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Dihydrocoumarin	5.89%
Dimethyl Anthranilate	1.32%
Dimethyl Sulfide	5.02%
Dodecane	0.74%
Ethanol*	23.12%
Ethyl-3-Hydroxy Butyrate	0.48%
Ethyl 2-Methyl Butyrate	15.99%
Ethyl 2-Phenyl Acetate	1.41%
Ethyl Acetate	23.23%
Ethyl Acetoacetate	3.27%
Ethyl Butyrate	28.37%
Ethyl Cinnamate	1.50%
Ethyl Decanoate	1.63%
Ethyl Dodecanoate	0.84%
Ethyl Heptanoate	2.00%
Ethyl Hexanoate	13.56%
Ethyl Isovalerate	9.51%
Ethyl Lactate	3.60%
Ethyl maltol	32.01%
Ethyl menthane carboxamide	1.51%
Ethyl methyl phenylglycidate	2.41%
Ethyl Nonanoate	1.50%
Ethyl Octanoate	2.26%
Ethyl Propionate	10.94%
Ethyl Vanillin	19.38%
Ethyl Vanillin Propylene Glycol Acetal	0.32%
Eucalyptol	3.00%
Eugenol	6.01%
Fenugreek	1.62%
Furaneol	19.31%
Furfural	2.98%
Furfuryl Alcohol	2.32%
gamma-Decalactone	18.16%
gamma-Dodecalactone	2.99%
gamma-Hexalactone	5.10%
gamma-Nonalactone	9.53%
gamma-Octalactone	7.27%
gamma-Terpinene	0.82%
gamma-Undecalactone	10.86%
gamma-Valerolactone	0.74%
Geranial	0.80%
Geraniol	4.06%
Geranyl acetate	3.51%
Ginger oil	0.14%
Glycerol*	94.14%
Glyceryl 1-acetate	0.91%
Guaiacol	6.05%
Hexanal	3.63%
Hexanoic Acid	11.10%
Hexyl Acetate	10.35%

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Hexyl Butyrate	1.71%
Ionone (mixed isomers)	0.99%
Isoamyl Acetate	16.33%
Isoamyl Alcohol	4.49%
Isoamyl Butyrate	6.83%
Isoamyl Isovalerate	11.46%
Isoamyl Phenyl Acetate	1.49%
Isobutyl Acetate	4.88%
Isobutyl Alcohol	1.41%
Isobutyl Butyrate	0.69%
Isobutyric Acid	0.50%
Isovaleraldehyde	1.78%
Jasmine Absolute	0.89%
L-Carvone	0.80%
Lactic Acid	3.42%
Lemon oil	6.35%
Levulinic Acid	0.81%
Lime oil	3.98%
Limonene	7.90%
Linalool	14.53%
Linalyl Acetate	3.41%
Maltol	22.76%
Mandarin Oil	0.50%
Menthol	12.10%
Menthone	2.92%
Methyl acetate	2.32%
Methyl-alpha-ionone	2.62%
Methyl Anthranilate	3.74%
Methyl Cinnamate	9.37%
Methyl cyclopentenolone	18.32%
Methyl dihydrojasmonate	0.81%
Methyl Salicylate	1.19%
Methyl Thiobutyrate	1.47%
Methyl trans-cinnamate	0.77%
Methyl-thio-methylpyrazine	2.45%
Myrcene	1.85%
n-Butanol	1.25%
n-Hexanol	3.58%
n-Octanal	1.10%
n-Propanol	0.51%
Neral	0.75%
Nerol	1.24%
Neryl Acetate	1.59%
Nicotine*	88.41%
Octanoic Acid	4.39%
Octanol	0.74%
Oleic Acid	1.09%
Orange oil	3.72%
p-Cymene	0.96%
Peppermint Oil	1.78%

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Peru Balsam	1.16%
Piperonal	9.56%
Potassium Sorbate	1.12%
Propenyl Guaethol	2.42%
Propionic Acid	4.27%
Propyl Acetate	0.33%
Propylene Glycol*	85.78%
Sodium Benzoate	1.16%
Sodium Citrate	1.16%
Spearmint oil	1.07%
Strawberry Extract	1.59%
Sucralose	8.25%
Sugar	1.26%
Tabanone	0.53%
Terpinolene	0.84%
Thio Menthone	1.62%
trans-2-Hexenal	3.85%
trans-2-Hexenoic acid	1.31%
trans-2-Hexenol	1.82%
trans-2-Hexenylacetaat	0.94%
trans-Anethole	2.19%
Triacetin*	14.44%
Triethyl Citrate	4.10%
Vanilla Extract	0.79%
Vanillin	35.17%
Vanillin Propylene Glycol Acetal	1.33%
Veratraldehyde	1.70%
Water*	44.96%

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### Supplementary Table S2

**Table S2:** An overview of all flavorings added to more than 10% of the e-liquids within a flavor category [1]. Prevalence is reported as the number of e-liquids containing the respective flavoring as percentage of the total number of e-liquids. The final column shows the median concentration of the flavoring ingredient for the respective flavor category. The 29 “category-specific” flavorings that were added to more than 10% of the e-liquids in a single category are marked in grey.

Category	Flavorings added to >10% of the e-liquid within the respective flavor category	Prevalence (% of total e-liquids)	Median concentration (mg/10mL)
<b>Tobacco</b> (8 flavorings)	Ethyl maltol	31.2%	6.78
	Methyl cyclopentenolone	29.6%	1.50
	Vanillin	25.9%	4.11
	2,3,5-Trimethylpyrazine	15.8%	1.32
	Furaneol	13.1%	2.97
	<b>β-Damascone</b>	12.6%	1.10
	2-Acetylpyrazine	12.3%	1.32
	Benzyl Alcohol	10.3%	6.00
<b>Menthol/mint</b> (6 flavorings)	Menthol	58.6%	57.60
	<b>Menthone</b>	16.6%	22.68
	Ethyl maltol	12.7%	0.74
	Vanillin	11.9%	1.24
	<b>Eucalyptol</b>	11.5%	7.15
	<b>Peppermint Oil</b>	11.4%	9.87
<b>Nuts</b> (32 flavorings)	Vanillin	58.8%	30.63
	Ethyl maltol	47.5%	24.50
	Ethyl Vanillin	35.0%	32.00
	Acetoin	27.5%	24.00
	Maltol	26.9%	6.17
	2,3-Pentanedione	23.8%	24.00
	Methyl cyclopentenolone	23.8%	24.00
	Butyric Acid	22.5%	24.00
	δ-Decalactone	22.5%	6.43
	γ-Decalactone	22.5%	1.63
	Ethyl Acetate	21.9%	24.00
	Ethyl Butyrate	21.9%	24.00
	Acetic Acid	21.3%	24.00
	Furaneol	20.0%	28.56
	Anisaldehyde	19.4%	24.00
	Guaiacol	19.4%	24.00
	δ-Dodecalactone	17.5%	1.63
	2,3,5-Trimethylpyrazine	16.9%	1.10
	Ethyl Propionate	16.9%	24.00
	2-Acetylpyrazine	15.6%	10.48
Butyl Butyryl Lactate	15.6%	50.91	
γ-Octalactone	15.0%	35.14	
<b>2,5-Dimethylpyrazine</b>	13.8%	0.56	
<b>4,5-Dimethyl-3-Hydroxy-2,5-</b>	11.9%	3.26	

	Dihydrofuran-2-One		
	5-Methyl Furfural	11.9%	4.63
	Benzyl Alcohol	11.9%	8.00
	Ethyl Lactate	11.9%	46.28
	$\gamma$ -Dodecalactone	11.9%	1.63
	Triethyl Citrate	11.9%	46.28
	Piperonal	10.6%	9.00
	Veratraldehyde	10.6%	2.17
	2-3-Hexanedione	10.0%	1.63
<b>Spices</b> (9 flavorings)	Menthol	23.5%	20.42
	Anethole	22.8%	60.00
	Ethyl maltol	22.8%	17.72
	Ethyl Butyrate	13.0%	2.49
	Benzyl Alcohol	11.7%	28.00
	Ethyl Vanillin	11.7%	27.37
	trans-Anethole	11.1%	105.00
	Vanillin	11.1%	30.60
	Anisaldehyde	10.5%	0.36
<b>Coffee/tea</b> (13 flavorings)	Vanillin	36.0%	5.68
	Methyl cyclopentenolone	21.4%	5.70
	Benzyl Alcohol	20.9%	17.00
	Ethyl maltol	15.3%	3.25
	Ethyl Vanillin	15.0%	2.47
	Furaneol	15.0%	2.35
	Maltol	15.0%	3.00
	$\delta$ -Decalactone	14.3%	0.60
	Acetic Acid	13.3%	0.66
	$\delta$ -Dodecalactone	11.6%	0.55
	Ethyl Acetate	11.6%	0.47
	Dihydrocoumarin	11.1%	0.97
	Ethyl Butyrate	11.1%	1.28
<b>Alcohol</b> (22 flavorings)	Vanillin	50.3%	9.00
	Ethyl Acetate	25.7%	7.92
	Ethyl Butyrate	23.1%	5.98
	Ethyl Propionate	18.8%	15.00
	Ethyl Heptanoate	18.5%	2.23
	Ethyl maltol	17.6%	10.85
	Benzaldehyde	16.5%	6.00
	$\gamma$ -Nonalactone	15.6%	5.62
	Ethyl Hexanoate	15.3%	0.90
	Acetic Acid	15.0%	1.58
	Maltol	14.2%	4.90
	Allyl Hexanoate	13.9%	2.33
	Piperonal	13.0%	1.14
	$\delta$ -Decalactone	12.7%	0.23
	Methyl cyclopentenolone	12.1%	10.82
	Isoamyl Alcohol	11.8%	0.61
	Isoamyl Acetate	11.3%	1.00
	Lactic Acid	11.3%	15.00
	Ethyl Vanillin	11.0%	9.41



	Ethyl Nonanoate	10.4%	1.00
	Furaneol	10.4%	7.96
	Menthol	10.1%	11.75
<b>Other beverages</b> (44 flavorings)	Vanillin	44.5%	7.19
	Ethyl Butyrate	39.6%	2.20
	Ethyl maltol	36.6%	3.23
	Ethyl Acetate	30.9%	0.75
	Ethyl Vanillin	30.8%	5.39
	Maltol	28.2%	0.90
	Isoamyl Acetate	26.4%	1.75
	Ethyl 2-Methyl Butyrate	25.5%	0.25
	Furaneol	25.0%	0.66
	Ethyl Hexanoate	23.7%	0.37
	Linalool	23.5%	0.31
	Methyl Cinnamate	22.0%	0.18
	Cis-3-hexenol	21.9%	1.00
	$\gamma$ -Decalactone	20.6%	0.25
	Butyric Acid	20.3%	0.26
	Ethyl Isovalerate	20.2%	0.90
	Acetic Acid	19.4%	0.14
	Benzyl Acetate	18.5%	1.00
	Isoamyl Isovalerate	17.6%	0.20
	Benzaldehyde	17.2%	0.19
	Lemon oil	17.2%	6.10
	Benzyl Alcohol	16.0%	2.82
	Sucralose	16.0%	8.84
	Citral	15.1%	0.61
	Methyl cyclopentenolone	14.5%	0.46
	Isoamyl Butyrate	14.2%	1.64
	$\beta$ -Ionone	13.8%	0.75
	Eugenol	13.8%	1.97
	Ethyl Propionate	13.6%	0.48
	Hexanoic Acid	13.6%	0.26
	$\gamma$ -Undecalactone	13.5%	0.41
	4-(4-Hydroxyphenyl)-2-butanone	13.2%	3.11
	Lime oil	13.1%	27.50
	Alpha-Ionone	12.9%	1.00
	alpha-Terpineol	12.9%	0.74
	Cinnamaldehyde	12.5%	3.31
	Limonene	12.5%	4.50
	Cis-3-hexenyl Acetate	12.3%	0.14
	Piperonal	11.9%	0.20
	Hexyl Acetate	11.4%	0.60
	Allyl Hexanoate	10.9%	1.00
	Anisaldehyde	10.6%	0.11
	$\gamma$ -Nonalactone	10.3%	0.76
	2-Methyl Butyric Acid	10.2%	0.17
<b>Fruit (berries)</b> (36 flavorings)	Ethyl Butyrate	52.4%	6.21
	Cis-3-hexenol	41.2%	2.33
	Vanillin	39.1%	3.05

Furaneol	36.8%	3.26
Ethyl Acetate	36.0%	1.36
Ethyl 2-Methyl Butyrate	35.7%	2.51
Acetic Acid	33.5%	2.31
Ethyl maltol	33.5%	3.34
$\gamma$ -Decalactone	33.1%	0.91
Maltol	32.7%	1.21
4-(4-Hydroxyphenyl)-2-butanone	32.6%	1.78
Linalool	31.1%	0.92
Hexanoic Acid	26.3%	0.60
2-Methyl Butyric Acid	25.7%	2.79
Butyric Acid	25.5%	0.85
Ethyl Hexanoate	24.2%	0.81
Ethyl Isovalerate	23.8%	0.65
Methyl Cinnamate	23.4%	0.92
Isoamyl Acetate	22.0%	1.00
Cis-3-hexenyl Acetate	21.5%	1.00
Benzyl Acetate	19.6%	0.74
$\gamma$ -Undecalactone	19.1%	0.21
Benzyl Alcohol	19.0%	1.02
Hexyl Acetate	18.7%	0.41
Ethyl Vanillin	18.6%	2.92
$\beta$ -Ionone	17.4%	0.36
Ethyl Propionate	17.1%	0.32
Benzaldehyde	16.1%	0.15
Alpha-Ionone	16.0%	0.40
Menthol	15.7%	9.12
Dimethyl Sulfide	14.1%	0.20
Isoamyl Isovalerate	13.1%	0.96
Isoamyl Butyrate	12.8%	0.36
$\delta$ -Decalactone	11.6%	0.13
Sucralose	11.3%	12.15
Propionic Acid	11.0%	3.00
<b>Fruit (citrus)</b> <i>(31 flavorings)</i>		
Ethyl maltol	32.9%	5.98
Ethyl Butyrate	31.1%	2.85
Vanillin	31.0%	6.00
Ethyl Acetate	26.3%	0.66
Linalool	25.8%	1.56
Citral	23.4%	2.81
Lemon oil	21.9%	12.00
Maltol	20.3%	0.48
Ethyl Vanillin	19.9%	16.00
Lime oil	19.4%	9.66
alpha-Terpeneol	19.0%	0.26
Furaneol	18.4%	1.50
Cis-3-hexenol	17.6%	0.77
Limonene	17.1%	13.00
Orange oil	16.1%	1.74
$\gamma$ -Decalactone	15.9%	0.24
Benzyl Alcohol	15.3%	1.20

Methyl cyclopentenolone	14.9%	8.57
Ethyl Hexanoate	14.7%	2.62
$\delta$ -Dodecalactone	14.1%	1.13
Ethyl 2-Methyl Butyrate	13.1%	0.75
Acetic Acid	12.7%	1.10
Sucralose	12.4%	13.88
$\gamma$ -Nonalactone	12.1%	2.05
Ethyl Propionate	11.1%	1.30
4-(4-Hydroxyphenyl)-2-butanone	10.6%	1.00
Butyric Acid	10.3%	0.10
Hexanoic Acid	10.3%	0.68
Isoamyl Isovalerate	10.3%	0.67
2-Methyl Butyric Acid	10.2%	2.64
Ethyl Isovalerate	10.0%	0.20
<b>Fruit (tropical)</b>		
<i>(39 flavorings)</i>		
Ethyl Butyrate	38.5%	2.42
Vanillin	36.5%	2.75
Isoamyl Acetate	32.0%	2.25
Ethyl Acetate	31.2%	1.09
Ethyl maltol	30.7%	1.31
Cis-3-hexenol	29.1%	1.00
Ethyl Hexanoate	27.2%	0.72
Furaneol	26.2%	0.72
Maltol	24.9%	1.04
$\gamma$ -Decalactone	23.8%	0.49
Allyl Hexanoate	22.8%	1.11
Acetic Acid	21.8%	1.20
Ethyl 2-Methyl Butyrate	19.7%	1.47
Ethyl Vanillin	19.6%	1.78
$\gamma$ -Undecalactone	19.2%	0.33
Isoamyl Isovalerate	19.2%	1.10
Butyric Acid	18.7%	1.02
Benzyl Alcohol	18.4%	2.73
$\gamma$ -Nonalactone	18.4%	0.78
Benzaldehyde	17.6%	0.20
Isoamyl Butyrate	15.8%	1.54
Benzyl Acetate	15.4%	0.24
Methyl cyclopentenolone	15.4%	0.33
Limonene	15.3%	2.99
Hexanoic Acid	15.2%	0.40
Ethyl Propionate	15.0%	0.37
$\gamma$ -Octalactone	14.7%	0.42
Linalool	14.7%	0.40
Ethyl Isovalerate	14.4%	0.25
2-Methyl Butyric Acid	13.4%	1.40
Lemon oil	13.4%	0.25
Cis-3-hexenyl Acetate	12.7%	1.00
Hexyl Acetate	12.7%	0.83
Methyl Cinnamate	12.2%	0.20
Sucralose	11.8%	8.98
$\delta$ -Decalactone	11.4%	0.24

	Eugenol	11.2%	2.63
	Piperonal	11.1%	0.44
	Acetoin	10.5%	1.00
<b>Fruit (other) (35 flavorings)</b>	Ethyl Butyrate	42.6%	3.78
	Ethyl Acetate	37.7%	3.08
	Isoamyl Acetate	35.9%	3.57
	Vanillin	32.0%	2.81
	Maltol	28.1%	1.41
	Ethyl maltol	28.0%	0.95
	Ethyl 2-Methyl Butyrate	25.8%	1.49
	Hexyl Acetate	25.8%	1.16
	Cis-3-hexenol	25.7%	1.17
	Benzaldehyde	24.1%	1.45
	$\gamma$ -Decalactone	22.4%	0.29
	Acetic Acid	20.5%	1.21
	Linalool	19.9%	0.88
	$\gamma$ -Undecalactone	19.8%	0.77
	Furaneol	18.6%	1.00
	Ethyl Hexanoate	17.9%	0.24
	Cis-3-hexenyl Acetate	17.7%	0.51
	Benzyl Alcohol	15.3%	1.40
	Benzyl Acetate	14.6%	1.00
	Ethyl Vanillin	14.3%	1.88
	Ethyl Isovalerate	13.9%	1.20
	Isobutyl Acetate	13.7%	1.76
	Butyric Acid	13.2%	0.32
	trans-2-Hexenal	12.9%	1.93
	2-Methyl Butyric Acid	12.0%	1.34
	Ethyl Propionate	11.9%	0.33
	4-(4-Hydroxyphenyl)-2-butanone	11.7%	1.43
	Isoamyl Isovalerate	11.7%	0.77
	$\delta$ -Decalactone	11.0%	0.20
	Methyl cyclopentenolone	10.7%	0.50
	$\beta$ -Ionone	10.5%	0.13
	Limonene	10.5%	1.77
	Anisaldehyde	10.3%	0.92
	Menthol	10.3%	16.59
	Sucralose	10.2%	10.80
<b>Dessert (47 flavorings)</b>	Vanillin	74.5%	21.80
	Ethyl maltol	64.8%	9.02
	Ethyl Vanillin	63.0%	13.76
	Maltol	50.9%	1.37
	Methyl cyclopentenolone	49.2%	1.20
	Butyric Acid	45.7%	1.00
	Ethyl Butyrate	44.4%	1.40
	$\gamma$ -Decalactone	40.6%	0.24
	$\delta$ -Decalactone	39.5%	0.36
	Ethyl Acetate	38.7%	0.39
	Furaneol	34.2%	2.10
	$\gamma$ -Nonalactone	34.1%	0.96

Isoamyl Isovalerate	33.5%	0.51
Piperonal	33.1%	0.36
Anisaldehyde	31.8%	0.20
4-Methyl-5-Thiazole Ethanol	30.2%	0.35
Guaiacol	30.0%	0.24
Ethyl Propionate	29.9%	0.98
Anisyl Alcohol	29.4%	0.72
$\delta$ -Dodecalactone	29.0%	0.29
Benzyl Alcohol	28.8%	4.01
Hexanoic Acid	27.4%	1.14
$\gamma$ -Octalactone	27.0%	0.54
Cis-3-hexenol	25.0%	1.00
$\gamma$ -Hexalactone	24.8%	0.54
Acetoin	24.0%	1.36
Ethyl 2-Methyl Butyrate	22.2%	1.51
Sucralose	21.8%	8.68
Acetic Acid	21.3%	0.44
Dihydrocoumarin	21.3%	1.00
2-Acetylpyrazine	20.5%	1.26
Benzaldehyde	20.0%	0.10
Ethyl Hexanoate	17.6%	0.62
Linalool	17.2%	0.79
2-Methyl Butyric Acid	16.4%	1.18
Methyl Cinnamate	14.7%	1.00
Butyl Butyryl Lactate	13.7%	1.01
2,3-Pentanedione	13.3%	1.17
$\gamma$ -Undecalactone	13.3%	0.67
Benzyl Benzoate	13.1%	0.46
Isoamyl Acetate	13.1%	2.20
Methyl-alpha-ionone	12.8%	1.77
Ethyl Lactate	12.6%	0.67
Methyl-thio-methylpyrazine	11.9%	0.06
$\beta$ -Ionone	11.1%	0.42
Hexyl Acetate	10.8%	0.60
Propenyl Guaethol	10.2%	1.00
<b>Candy</b> (34 flavorings)		
Ethyl maltol	39.4%	0.50
Isoamyl Acetate	37.4%	2.29
Ethyl Butyrate	37.2%	1.13
Vanillin	35.2%	1.07
Ethyl Acetate	35.0%	0.39
Maltol	26.2%	0.50
Cis-3-hexenol	23.2%	1.00
Ethyl 2-Methyl Butyrate	22.9%	0.17
Ethyl Vanillin	21.6%	0.28
Linalool	21.0%	0.66
Butyric Acid	20.5%	0.32
Ethyl Hexanoate	20.1%	0.11
$\gamma$ -Decalactone	19.9%	0.24
Ethyl Isovalerate	19.5%	0.17
Benzaldehyde	17.9%	0.10

Furaneol	17.6%	1.21
Benzyl Acetate	17.3%	1.00
4-(4-Hydroxyphenyl)-2-butanone	17.0%	1.00
Benzyl Alcohol	16.7%	0.68
$\gamma$ -Undecalactone	16.0%	0.20
Hexyl Acetate	16.0%	1.00
Isoamyl Butyrate	15.7%	1.28
Isoamyl Isovalerate	14.8%	0.39
Methyl Cinnamate	13.9%	0.18
Methyl cyclopentenolone	13.3%	0.14
Hexanoic Acid	12.9%	0.22
2-Methyl Butyric Acid	12.6%	0.30
Citral	12.3%	0.75
Acetic Acid	12.2%	0.40
$\beta$ -Ionone	12.0%	0.66
Cis-3-hexenyl Acetate	11.4%	0.26
Ethyl Propionate	10.6%	0.20
Eugenol	10.6%	0.45
Lemon oil	10.4%	0.13
<hr/>		
<b>Other sweets</b>		
(20 flavorings)		
Vanillin	61.4%	30.00
Ethyl maltol	37.5%	28.04
Ethyl Vanillin	35.0%	19.68
Maltol	26.0%	1.30
Piperonal	24.4%	3.18
Methyl cyclopentenolone	22.0%	5.65
$\delta$ -Decalactone	18.9%	0.71
Ethyl Butyrate	18.6%	0.51
$\gamma$ -Nonalactone	16.2%	0.75
Furaneol	15.1%	2.22
Isoamyl Isovalerate	13.7%	1.11
2,3,5-Trimethylpyrazine	13.1%	0.25
Anisaldehyde	13.1%	0.50
Ethyl Acetate	13.0%	0.57
$\gamma$ -Decalactone	12.9%	0.30
Butyric Acid	12.6%	0.77
Acetoin	12.0%	1.15
Guaiacol	11.1%	0.04
$\delta$ -Dodecalactone	10.0%	0.40
Veratraldehyde	10.0%	2.96
<hr/>		
<b>Other flavors</b>		
(34 flavorings)		
Linalool	30.5%	3.00
Ethyl Butyrate	25.2%	6.00
Ethyl Acetate	23.2%	8.00
Maltol	23.2%	4.10
Ethyl 2-Methyl Butyrate	22.5%	5.90
Vanillin	21.9%	21.00
Acetic Acid	21.2%	0.70
Isoamyl Acetate	20.5%	6.00
Cis-3-hexenyl Acetate	19.2%	0.30
Cis-3-hexenol	18.5%	1.80
Ethyl Acetoacetate	18.5%	0.20

	Ethyl Hexanoate	18.5%	0.20
	Butyric Acid	17.2%	1.95
	Hexyl Acetate	17.2%	8.00
	Isoamyl Butyrate	17.2%	5.20
	Cis-3-Hexenyl Butyrate	15.2%	0.10
	Ethyl Isovalerate	15.2%	0.10
	$\gamma$ -Decalactone	15.2%	1.20
	Hexanal	15.2%	0.02
	Linalyl Acetate	15.2%	0.04
	Furaneol	13.9%	7.40
	Myrcene	13.2%	25.60
	Anisaldehyde	12.6%	1.80
	Dihydrocoumarin	12.6%	30.00
	Ethyl maltol	12.6%	17.70
	Limonene	12.6%	6.97
	2-Phenylethanol	11.9%	0.10
	Citronellol	11.9%	6.00
	2-Methyl Butyric Acid	11.3%	1.10
	Benzaldehyde	11.3%	6.60
	$\beta$ -Caryophyllene	11.3%	25.60
	Hexanoic Acid	11.3%	0.20
	Methyl Cinnamate	11.3%	0.40
	$\beta$ -Damascenone	10.6%	0.10
<b>Unflavored</b> (0 flavorings)	NA	NA	NA

## Supplementary Table S3

**Table S3:** Flavor descriptions, retrieved from a commercial flavor database [2], of the ingredients listed in the main text of the manuscript. Ingredients are presented in alphabetical order.

Flavoring ingredient	Flavor description	Flavor category that the ingredient is specific to (category-specific flavorings)*
2,3,5-Trimethylpyrazine	Baked potato, roasted nut, cocoa, coffee, burnt	
2,5-Dimethylpyrazine	Chocolate, roasted nuts, earthy	Nuts
2-3-Hexanedione	Creamy, sweet buttery odor & butter-cheese, fruity, caramellic taste	Nuts
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one	Powerful caramel aroma; sweet burnt taste	Nuts
4-Methyl-5-thiazole ethanol	In dilution, meaty-beef like with nutty note	Dessert
5-Methyl furfural	Sweet spicy, bready, nutty, caramellic	Nuts
Acetic acid <sup>o</sup>	Pungent, sour, acid, vinegar	
Acetoin	Creamy-buttery, yogurt-like	
Anethole	Sweet, herbaceous, anise (artificial licorice)	Spices
Anisyl alcohol	Sweet, fruity, floral, balsamic anisic-vanilla-creamy-coumarinic like	Dessert
Benzaldehyde <sup>o</sup>	Bitter almond oil, sweet cherry	
Benzyl alcohol <sup>o</sup>	Faint, sweet, almond fruity, somewhat chemical	
Benzyl benzoate	Faint, sweet, balsamic with slight bitter, fruity notes	Dessert
Butyric acid <sup>o</sup>	Tropical fruity floral, plum, apricot-pear-like	
Cinnamaldehyde	Spicy, cinnamon-cassia-like with sweet warm (hot) taste	Other beverages
Cis-3-hexenol <sup>o</sup>	Strong, fresh, green, grassy	
δ-Decalactone <sup>o</sup>	Sweet, creamy, milky, peach, nut, buttery	
Dimethyl sulfide	Pungent, cabbage, cooked vegetable odor; corn-like on dilution	Fruit, berries
Ethyl 2-methyl butyrate <sup>o</sup>	Strong, green, fruity, apple with strawberry notes	
Ethyl acetate <sup>o</sup>	Ethereal, sharp, wine-brandy-like	
Ethyl butyrate <sup>o</sup>	Ethereal, fruity with buttery-pineapple-banana, ripe fruit & juicy notes	
Ethyl heptanoate	Strong, fruity, winey, cognac-like	Alcohol
Ethyl hexanoate <sup>o</sup>	Strong, fruity, pineapple, banana with strawberry, pear & tropical notes	
Ethyl maltol <sup>o</sup>	Sweet, fruity-caramellic, cotton candy	
Ethyl nonanoate	Fatty-waxy, oily, wine-cognac, grape, tropical, nut-like	Alcohol
Ethyl propionate <sup>o</sup>	Strong, ethereal, fruity, rum-like	
Ethyl vanillin <sup>o</sup>	Intense, sweet, creamy, vanilla-like	
Eucalyptol	Strong, camphoraceous, cool, fresh	Menthol/mint
Furaneol <sup>o</sup>	Fruity, caramelized, roasted, pineapple-strawberry	
Hexanoic acid <sup>o</sup>	Heavy, fatty, cheesey-sweaty	
Hexyl acetate <sup>o</sup>	Sweet, fruity, pear-apple, green, banana	
Isoamyl acetate <sup>o</sup>	Sweet, fruity, banana, pear	
Isoamyl alcohol	Breathtaking, alcoholic odor; in dilution a winey-brandy taste	Alcohol
Isoamyl isovalerate <sup>o</sup>	Fruity, green-apple, pineapple, tropical, mango, apricot, cognac	
Isobutyl acetate	Fruity, banana-apple-pear-pineapple	Fruit, other
Lactic acid	Weak, sour, buttermilk	Alcohol
Linalool <sup>o</sup>	Sweet floral-woody with slight citrus notes	
Maltol <sup>o</sup>	Sweet, fruity, berry, strawberry, caramellic	
Menthol <sup>o</sup>	String trigeminal cooling sensation with a slight mint note	



Menthone	Minty-herbaceous (not green); dry woody notes	<i>Menthol/mint</i>
Methyl cyclopentenolone <sup>o</sup>	Very strong, caramellic-maple, lovage	
Methyl-alpha-ionone	Orris, violet, woody, floral, oily with woody raspberry notes	<i>Dessert</i>
Methyl-thio-methyl-pyrazine	Roasted nut, burnt, meaty	<i>Dessert</i>
Orange oil	Orange	<i>Fruit, citrus</i>
Peppermint oil	Peppermint	<i>Menthol/mint</i>
Piperonal	Sweet, floral-cherry (heliotrope); sweet cherry-vanilla taste	
Propenyl guaethol	Sweet, vanilla, creamy, phenolic, anisic flavor	<i>Dessert</i>
Propionic acid	Pungent, sour milk, cheese	<i>Fruit, berries</i>
Trans-2-hexenal	Green, fruity, fresh, apple with leafy and grassy notes	<i>Fruit, other</i>
Trans-anethole	Sweet, herbaceous, anise (artificial licorice)	<i>Spices</i>
Triethyl citrate	Weak, sweet, winey-fruity-plum-like odor; slight bitter taste	<i>Nuts</i>
Vanillin <sup>o</sup>	Sweet, powerful, creamy, vanilla-like	
$\beta$ -damascone	Blackcurrant, plum, rose, honey, tobacco	<i>Tobacco</i>
$\gamma$ -Decalactone <sup>o</sup>	Coconut-peach	
$\gamma$ -Dodecalactone	Fatty, fruity, peach odor	<i>Nuts</i>
$\gamma$ -Hexalactone	Coumarin-like, sweet, creamy note	<i>Dessert</i>
$\gamma$ -Undecalactone <sup>o</sup>	Strong fatty, peach-apricot	

\* A flavoring ingredient added to more than 10% of the e-liquids in a single category was considered “category-specific”.

<sup>o</sup> The 25 flavoring ingredients that were most frequently added to e-liquids from the EU-CEG dataset. These data are also presented in Table 1 of the main manuscript.

## Supplementary Table S4

**Table S4:** Prediction accuracy of a random forest (RF) algorithm that assigns e-liquids a flavor category [1] based on information about flavoring composition. Actual category is the flavor category where we classified the product in based on flavor-related information from the EU-CEG system.

Category	Description	Predicted category																Total	Predicted correctly	Predicted at 2 <sup>nd</sup> place	Remaining
		Cat01	Cat02	Cat03	Cat04	Cat05	Cat06	Cat07	Cat08	Cat09	Cat10	Cat11	Cat12	Cat13	Cat14	Cat15	Cat16				
Cat01	tobacco	2323	22	0	0	0	0	1	2	0	1	8	11	0	18	0	0	2386	2323 (97%)	41 (2%)	22 (1%)
Cat02	menthol/mint	336	726	0	0	0	0	1	3	3	0	2	4	0	1	0	0	1076	726 (67%)	324 (30%)	26 (2%)
Cat03	nuts	64	3	54	0	0	0	0	0	0	2	4	13	0	20	0	0	160	54 (34%)	58 (36%)	48 (30%)
Cat04	spices	75	6	0	67	0	0	1	3	0	0	1	9	0	0	0	0	162	67 (41%)	79 (49%)	16 (10%)
Cat05	coffee/tea	213	0	0	0	163	0	0	0	4	4	4	13	0	5	0	0	406	163 (40%)	208 (51%)	35 (9%)
Cat06	alcohol other beverages	112	3	0	0	2	197	1	2	5	1	7	10	0	6	0	0	346	197 (57%)	124 (36%)	25 (7%)
Cat07	fruit (berries)	189	1	0	0	1	4	512	15	9	5	8	26	0	3	0	0	773	512 (66%)	219 (28%)	42 (5%)
Cat08	fruit (citrus) fruit (tropical)	431	13	0	0	0	0	4	1392	1	5	13	25	1	11	0	0	1896	1392 (73%)	462 (24%)	42 (2%)
Cat09	fruit (other)	189	9	0	0	0	0	9	24	413	6	1	6	0	2	0	0	659	413 (63%)	213 (32%)	33 (5%)
Cat10	dessert	293	5	0	0	0	0	2	13	5	639	15	14	1	6	0	0	993	639 (64%)	307 (31%)	47 (5%)
Cat11	candy	586	20	0	0	1	3	4	22	15	7	1476	25	1	3	0	0	2163	1476 (68%)	610 (28%)	77 (4%)
Cat12	other sweets	270	2	0	0	6	2	1	6	11	2	17	1140	0	28	0	0	1485	1140 (77%)	314 (21%)	31 (2%)
Cat13	other flavors	209	12	1	5	0	0	0	20	2	4	17	14	398	0	0	0	682	398 (58%)	256 (38%)	28 (4%)
Cat14	unflavored	208	5	4	0	0	0	1	4	0	1	8	35	0	411	0	0	677	411 (61%)	232 (34%)	34 (5%)
Cat15	unclassifiable	60	3	0	0	0	0	0	1	5	0	3	8	0	6	65	0	151	65 (43%)	61 (40%)	25 (17%)
Cat16		232	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	238	6 (3%)	232 (97%)	0 (0%)
Cat17		1447	189	3	3	14	67	27	232	51	41	257	173	4	74	4	0	2586	NA	NA	NA
	Total	7237	1019	62	75	187	273	564	1739	524	718	1841	1526	405	594	69	6	16839	9982 (70%)	3740 (26%)	531 (4%)

**References**

- [1] Krusemann EJZ, Boesveldt S, de Graaf K, *et al.* An E-liquid Flavor Wheel: A Shared Vocabulary based on Systematically Reviewing E-liquid Flavor Classifications in Literature. *Nicotine Tob Res* 2018.
- [2] Leffingwell & Associates. Flavor-Base 9 - Tobacco Version for Windows XP/Vista/7&8. 2013.