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The pyrolysis of non-volatile tobacco ingredients using a system that simulates cigarette combustion conditions

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Abstract

This is the second part of a systematic study in which tobacco ingredients are pyrolysed using experimental conditions designed to simulate the average combustion conditions inside a burning cigarette. In the first part, the pyrolysis system was developed and single-substance, mostly semi-volatile tobacco ingredients were pyrolysed. It was predicted that on a cigarette, the majority of these semi-volatile ingredients would transfer to smoke with little pyrolysis.

In this part of the study, a further 159 non-volatile and complex ingredients, as well as ingredient mixtures, have been pyrolysed and the pyrolysis products determined using a gas chromatography–mass spectrometric system coupled to the pyrolyser. These non-volatile tobacco ingredients generally decomposed completely in the pyrolysis system, often yielding many products in relatively small amounts. The study has concentrated on the biologically active substances produced by pyrolysis, in particular the ''Hoffmann analytes''. These analytes are believed by regulatory authorities in Canada and U.S.A. to be relevant to smoking-related diseases. They are based on lists published by Hoffmann and co-workers of the American Health Foundation in New York. For the pyrolysis of many of the non-volatile ingredients, no ''Hoffmann analytes'' were detected amongst the products. When they were occasionally formed, they included phenols, benzene, toluene, styrene and furfural (furfural is biologically active but it does not appear on any of the Hoffmann or regulatory authority lists). Those ingredients that did yield such products generally produced them in relatively small quantities although furfural was produced in relatively large quantities by pyrolysis of some ingredients, especially sugars. Those ingredients that produced biologically active constituents during their pyrolysis have been further assessed. This was done by adding them to cigarettes, machine-smoking the cigarette and comparing their smoke yields to those from a control (no ingredient) cigarette. From this comparison, it was found that in general the ingredients added to cigarettes do not increase the smoke components relative to the control cigarette. The pyrolysis technique of the present study tends to over-predict the amount of decomposition that the non-volatile ingredients undergo relative to their behaviour in a burning cigarette. Several examples are discussed, in particular ingredients that produce furfural during pyrolysis.

This general pyrolysis technique is thus a first step in the total toxicological assessment of tobacco ingredients and is a useful screening tool for indicating which ingredients may yield biologically active products during decomposition of the ingredients. There are, however, some products such as formaldehyde and the carbon oxides that are not detected by the pyrolyser-gas chromatography–mass spectrometric technique employed here. The generation and detection of these products during the pyrolysis of selected tobacco ingredients is the subject of a parallel paper.

Keywords: Burning; Cigarette; Combustion; Ingredient; Pyrolysis; Smoke; Tobacco; Mass spectrometer

1. Introduction

In some parts of the world, tobacco companies add ingredients to tobacco products, either to impart a specific taste, flavour or aroma to the product, or for a specific technological purpose such as increasing the moisture-holding capacity of the tobacco. Justification for the use of tobacco ingredients cannot be based solely on their approved use in food since, potentially, they could decompose into other substances during tobacco combustion in the smoking process [1]. The pyrolytic behaviour of the ingredient is a

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first step in its total toxicological assessment. It is used to predict whether the ingredient distils unchanged out of the cigarette-burning zone into smoke, or whether it decomposes into products, in particular those of toxicological concern. However, the experimental pyrolysis conditions must mimic as far as possible those that occur inside a burning cigarette during smoking, otherwise false predictions can be made [2,3].

In the first part of this study [3], a pyrolysis system was developed that simulated tobacco combustion in a burning cigarette. It was used to assess the behaviour of 291 single-substances, mostly semi-volatile tobacco ingredients. It was predicted that on a cigarette, the majority of these semi-volatile ingredients would transfer to smoke with little pyrolysis. In this second part of the study, the technique has been applied to 159 non-volatile and complex ingredients, as well as ingredient mixtures.

The results of the previous study indicated that the pyrolysis technique used gave good predictions of the smoke transfer/pyrolytic behaviour in a burning cigarette of relatively volatile tobacco ingredients. For non-volatile ingredients, the pyrolysis system gave over-estimates of the pyrolytic decomposition that occurs in the burning cigarette. It seems that in the experimental pyrolysis system, non-volatile substances remain in the high-temperature region longer than when they are part of the combustion matrix in a burning cigarette, and therefore are subjected to greater decomposition. Nevertheless, the pyrolysis technique is a useful screening tool for indicating which ingredients undergo significant decomposition during the smoking of cigarettes and determining whether products of toxicological concern are generated, which would warrant further smoke chemical assessment. Those non-volatile ingredients that do not generate such products in the pyrolysis system are unlikely to do so in a burning cigarette.

2. Experimental procedure

The experimental pyrolysis system was similar to that described previously [3]. Briefly, 20 μg of the ingredient was pyrolysed, usually in solution in ethanol, or about 2 mg of the solid when insoluble. The solution was microsyringed onto a piece of quartz wool (1 mg, approximately 2 mm long) contained in a quartz tube (2 mm i.d., 25 mm long). The quartz tube was placed in the pyroprobe, which was then inserted into a CDS Pyrolyser 2000 and sealed. The products of pyrolysis were separated using a capillary column in an Agilent 6890 gas chromatograph; their mass spectra detected with an Agilent 5973 mass spectrometer and identified using the Wiley library of mass spectra. The pyrolysis conditions were carefully chosen to simulate the average conditions inside the burning zone of the cigarette during smoking. Much is known about these conditions: extensive work conducted in the 1970s and 1980s showed that the cigarette-burning zone consists of two regions [4]. The exothermic combustion region has depleted oxygen levels, at or near zero throughout much of the combustion zone, temperatures varying from about 700 to 950 °C and tobacco heating rates up to 500 °C/s. Immediately downstream of the combustion region, the endothermic pyrolysis/distillation region has temperatures of about 100–600 °C, heating rates of about 10–50 °C/s and oxygen levels of 5–20 °C (v/v). Thus, the pyrolysis conditions used in the present study included a flowing atmosphere of 9% oxygen in nitrogen through the pyrolysis unit (the mean oxygen concentration inside the cigarette-burning zone), initially holding the pyroprobe at 300 °C for 5 s (to stimulate the interpuff smoulder period), then heating at 30 °C/s to 900 °C (mean heating rate and temperature range of cigarette-burning zone during a puff) and finally holding the temperature at 900 °C for 5 s (maximum duration of the high burning zone temperature during a puff under extreme human smoking conditions).

The substances pyrolysed were ‘‘food grade’’ materials, similar to the grade of the ingredient used commercially when added to tobacco as an ingredient. Each pyrolysis was carried out at least in duplicate. Before each set of replicates, the quartz tube and wool were analysed as a blank to ensure that there was no carryover between samples.

3. Results and discussion

3.1. Preliminary comments

The detailed results of the 159 ingredients pyrolysed in the present study are given in Appendix A. The percentages of products in the pyrolysate were calculated assuming all pyrolysis products had the same peak area/quantity relationships as the original ingredient being pyrolysed. The products were identified from the Wiley library of mass spectra. Some mass spectra were only identified tentatively and these are listed with a question mark after the name. Some products are also listed as a combination of substances, which may be either a genuine mixture or an indecision on identification. Contamination peaks due to ethanol solvent and column bleed were identified and removed from quoted products.

The composition of the pyrolysate is the mean of two pyrolyses for each ingredient. Generally, the variation between the replicates was less than 15%. Most, possibly all, of the non-volatile tobacco ingredients in this study decomposed completely in the pyrolysis system, often yielding many products in relatively small amounts. For each ingredient, the five most abundant products are listed in Appendix A. In addition, any products of known biological activity are also listed in Appendix A. These are generally those on the ‘‘Hoffmann list’’ of toxicological substances in cigarette smoke. These smoke analytes are believed by regulatory authorities in Canada and U.S.A. to be relevant to the development of smoking-related diseases [5,6]. They are

based on lists published by Hoffmann and co-workers of the American Health Foundation in New York, e.g. [7,8].

Many of the ingredients are listed in Appendix A by their names as commonly used by flavour chemists. In order to avoid any ambiguity, the Chemical Abstract Service (CAS) Registry Number for each ingredient is also listed. Further details of the botanical origins of the ingredient, processes used to extract them, and individual chemicals or types of chemicals in mixtures are given in Fenaroli's Handbook of Flavour Ingredients [10]. Several of the ingredients are listed as 'extracts' and 12 of these were extracted and diluted with glycerol and/or propylene glycol, e.g. apricot extract and carob bean extract. For these extracts, high levels of the extract solvent glycerol or propylene glycol were detected in the pyrolysate as indicated in Appendix A.

For seven ingredients, e.g. calcium carbonate, diammonium hydrogen phosphate and extracts such as tea extracts, no products were detected. The reasons for this are associated with the analytical system and/or the nature of the material being pyrolysed. Because of the characteristics of the gas chromatography–mass spectrometer detection system [3], water, CO, CO_2, NH_3 and products with a molecular weight below about 40 were not detected. Thus, the likely products from the pyrolysis of calcium carbonate (CO_2) and diammonium hydrogen phosphate (NH_3) would not be detected. Several of the materials pyrolysed are described as distillates, extracts or tinctures in Appendix A. These are the exact materials that would be used commercially as tobacco ingredients. Flavour extracts and tinctures have a high solvent content, often water and ethanol; flavour distillates from plant materials have high water content. The water must have dominated the pyrolysate such that other products were not detected.

From the detailed pyrolysis results given in Appendix A, an upper level for the maximum amount of each pyrolysis product in cigarette mainstream smoke when the ingredient was added to a cigarette has been calculated. The details of this calculation have been described elsewhere [3]. The calculation was for an unfiltered (plain) cigarette with the maximum ingredient application level, maximum tobacco weight in the cigarette, maximum proportion of tobacco burnt in puffing and 100% transfer of the ingredient and pyrolysis products to mainstream smoke. It was also assumed in the calculation that all the pyrolysis products were detected. This assumption is not correct for those ingredients that generate water, carbon dioxide, carbon monoxide or non-volatile ingredients that produce a solid char, for example. The maximum levels of pyrolysis products calculated in mainstream smoke are thus over-estimates in general, and probably large over-estimates for non-volatile ingredients.

In considering the contribution of the potential pyrolysis products from ingredients to total smoke, we have chosen to exclude, at this stage, any chemical predicted to be produced from the ingredient at less than 0.03 μg/cigarette. Thus, based on the assumption that a smoker consumes a maximum of 50 cigarettes a day, if a chemical from the ingredient were present in the smoke at 0.03 μg/cigarette, their daily intake of the chemical from the ingredient would be 1.5 μg. It has been reported that the intake of a chemical by ingestion from food at up to 1.5 μg/day is of no toxicological concern [11]. This is the basis of our cut-off of 0.03 μg/cigarette. It is realised that with smoking the chemical is inhaled and not ingested and so this is a first approximation. However, applying this model does offer a means of prioritising the data produced from pyrolysis studies of this type. This threshold model is applied solely to chemicals in smoke produced from ingredients and is not intended as a means of assessing the significance of smoke per se. We are not implying that levels of chemicals in smoke below 0.03 μg/cigarette are 'safe'. Indeed, epidemiology shows that the only way to avoid a smoking-related risk is not to smoke.

3.2. Pyrolysis to 'Hoffmann analyte' products

'Hoffmann analytes' [5–9] or other biologically active substances such as furfural [12] have been detected in the pyrolysates of 56 of the tobacco ingredients and these are highlighted in bold in Appendix A. These substances that are predicted to be in cigarette smoke from pyrolysis of the ingredient, at or above the threshold limit of 0.03 μg/cigarette, detailed in Appendix A, are listed in Table 1. Typical smoke levels reported for an unfiltered cigarette [4,7] are also included in Table 1 in order to compare the maximum ingredient contribution to smoke yields. Smoke data for unfiltered cigarettes are given in Table 1 in order to compare like with like, since the basis of the prediction is for an unfiltered cigarette.

From the data in Table 1 it is seen that, for some ingredients such as alfalfa extract and fenugreek extract, the maximum predicted levels of the biologically active pyrolysis products from tobacco ingredients are small compared to the typical levels in smoke. However, for other ingredients such as acacia powder, cellulose fibre and brown or white sugar, pyrolysis of the ingredient could generate maximum yields of biologically active products that far exceed the typical levels in smoke, particularly for furfural generation. The generalisation from the previous study [3] and summarised in Section 1 above is emphasised: for non-volatile ingredients the present pyrolysis system gives over-estimates of the pyrolytic decomposition that occurs in a burning cigarette. Nevertheless, the data presented in Table 1 have flagged tobacco ingredients that could potentially yield significant levels of biologically active pyrolysis products. The next step in the total assessment of the ingredients was to smoke cigarettes containing these ingredients to determine their effects on actual smoke yields. This has been done for the ingredients listed in Table 1, and mixtures of ingredients have been added, at or above their maximum levels, to a U.S. blended tobacco and made into filter cigarettes [13,14]. The cigarettes were then machine-

Table 1
Pyrolysis products from tobacco ingredients that are included in the "Hoffmann lists" or other lists of biologically active smoke components [5–9,12]

Ingredient (maximum cigarette level[a], ppm)	Pyrolysis product	Maximum level in smoke from ingredient (μg/cigarette)	Typical smoke levels[b] (μg/cigarette)
Acacia powder (15,000)	Furfural	240	15–43
	2-Butanone	38	30–100
Alfalfa extract (34)	Phenol	0.5	80–160
	Furfural	0.2	14–43
Ammonium glycyrrhizinate (52)	Phenol	2	80–160
	Cresol	1	11–37
	Toluene	0.7	100–200
Apple extract (200)	Furfural	6	15–43
Apricot extract (560)	Furfural	4	15–43
Brandy, absolute (40)	Furfural	0.04	15–43
Caramel (500)	Furfural	6	15–43
Carob bean extract (3400)	Furfural	26	15–43
Carob bean extract (roasted) (3400)	Furfural	5	15–43
Carob bean extract powder (7000)	Furfural	280	15–43
Catechu powder (1)	Phenol	0.06	80–160
Celery seed oleoresin (10)	Styrene	0.1	10–20
Cellulose fibre (17,000)	Furfural	410	15–43
	Benzene	260	20–70
	2-Butenal	220	10–20
	Phenol	180	80–160
	Toluene	85	100–200
	Cresol	77	11–37
	Styrene	60	10–20
Cherry juice (10)	Furfural	0.3	15–43
Chocolate (2700)	Phenol	15	80–160
	Toluene	12	100–200
	Benzene	7	20–70
	Cresol	7	11–37
	Pyridine	7	16–46
	Furfural	5	15–43
Cocoa powder (20,000)	Furfural	210	15–43
	Phenol	160	80–160
	Cresol	140	11–37
	2-Butanone	90	30
	Toluene	70	100–200
	Styrene	20	10–20
Cocoa shell extract (12,000)	Cresol	12	11–37
	Phenol	12	80–160
	Furfural	6	15–45
	Styrene	6	10–20
Coffee extract (100)	Pyridine	2	16–46
	Phenol	0.8	80–160
	Furfural	0.4	15–43
	Cresol	0.3	11–37
	Toluene	0.3	100–200
Coriander seed oil (560)	Styrene	0.3	10–20
Corn syrup (17,000)	Furfural	3850	15–43
	Phenol	30	80–160
Dextrin (1)	Furfural	0.1	15–43
Fenugreek extract (175)	Pyridine	0.4	16–46
	2-Butanone	0.3	30–100
	Benzene	0.2	20–70
	Toluene	0.2	100–200
	2-Butenal	0.09	10–20
	Furfural	0.09	15–43
Fenugreek tincture (500)	Pyridine	9	16–46
	Phenol	6	80–160

Table 1 (*Continued*)

Ingredient (maximum cigarette level[a], ppm)	Pyrolysis product	Maximum level in smoke from ingredient (μg/cigarette)	Typical smoke levels[b] (μg/cigarette)
	Furfural	1	15–43
Fig extract (800)	Furfural	98	15–43
d-Fructose (2100)	Furfural	80	15–43
Glucose (1300)	Furfural	35	15–43
Guar gum (2)	Furfural	0.06	15–43
Honey (34,000)	Furfural	4100	15–43
	Toluene	68	100–200
	Styrene	34	10–20
Honey absolute (30)	Furfural	2	15–43
Hydroxypropyl cellulose (3300)	Furfural	8	15–43
	Phenol	8	80–160
Kola nut extract (40)	Furfural	0.08	15–43
Licorice extract, powder (20,000)	Phenol	140	15–43
	Cresol	20	11–37
	Pyridine	20	16–46
	Furfural	20	15–43
Maple syrup (50)	Furfural	4	15–43
Oak chip extract (1)	Furfural	0.03	15–43
Orris root extract (40)	Phenol	0.2	80–160
Pectin (80)	Furfural	8	15–43
Pineapple extract (10)	Furfural	2	15–43
Pipsissewa leaves extract (10)	Furfural	0.3	15–43
Plum extract (40)	Furfural	0.08	15–43
	Styrene	0.08	10–20
Potassium citrate (10)	Benzene	0.4	20–70
	Toluene	0.4	100–200
	2-Butanone	0.4	30
Potassium sorbate (500)	Toluene	13	100–200
	Benzene	8	20–70
	Styrene	5	10–20
	Phenol	2	80–160
	2-Butanone	0.3	30
Prune juice concentrate (10,900)	Furfural	270	15–43
Raisin extract (10,000)	Furfural	620	15–43
	Benzene?	600	20–70
	Toluene	170	100–200
	Phenol	100	80–160
	Styrene	80	10–20
	Benzofuran	25	Present
	Cersol	25	11–37
	2-Butanone	20	30
	Pyridine	10	16–46
	2-Butenal	5	10–20
Sodium benzoate (5)	Benzene	2	20–70
	Phenol	0.04	80–160
Sodium citrate (5)	2-Butanone	0.1	30
	Cresol	0.05	11–37
	Toluene	0.05	100–200
Styrax extract (resinoid) (30)	Styrene	0.09	10–20
Sugar, brown (56,000)	Furfural	6200	15–43
Sugar, invert (62,000)	Furfural	11000	15–43
Sugar, white (25,000)	Furfural	4000	15–43
	Phenol	38	80–160
	Benzene	25	20–70
	Butanal?	13	40
	2-Butanone?	13	30–100
	Cresol	13	11–37
	Sryrene	13	10–20

Table 1 (*Continued*)

Ingredient (maximum cigarette level[a], ppm)	Pyrolysis product	Maximum level in smoke from ingredient (μg/cigarette)	Typical smoke levels[b] (μg/cigarette)
	Toluene	13	100–200
Valerian root extract (560)	Phenol	10	80–160
	Furfural	4	15–43
	Cresol?	1	11–37
Valerian root tincture (100)	Phenol	0.7	80–160
Vanilla, absolute (326)	Cresol	0.1	11–37
Vanilla oleoresin (326)	Phenol	0.2	80–160
Xantham gum (3800)	Furfural	46	15–43
	Phenol	15	80–160
	Cresol	10	11–37
	Toluene	8	100–200

[a] Typical maximum level used on British American Tobacco products.
[b] Typical smoke levels for an unfiltered cigarette [4,7]. The quoted butanal and 2-butanone ranges are for a filtered cigarette [12].

smoked under the standard ISO regime of one 35 ml puff of 2 s duration taken every minute. The yields of various constituents in mainstream smoke were determined using methods described previously [13]. The smoke yields of the biologically active products listed in Table 1 are given in Tables 2 and 3, relative to a control cigarette with no added ingredients. Mixtures of ingredients were added to the tobacco in the cigarettes depicted in Table 2; single ingredients were added to the tobacco in the cigarettes in Table 3. Further information on the ingredient mixtures is given in the detailed smoke chemistry papers [13,14]. Differences in yields of smoke analytes between the test and control cigarettes that are statistically significant are indicated in Tables 2 and 3. In the smoke chemistry studies, the analytical results obtained with a reference cigarette were found to vary over several months due to the variability of the analytical methodology for the low levels of smoke analytes being determined. When this long-term analytical variability was taken into account, some of the comparisons between the test and control cigarettes were found to no longer have statistically significant differences and this is also indicated in Table 2. (The nomenclature for the test cigarettes in Table 2, A2, A5, etc., is consistent with that used in the papers describing the smoke chemistry studies in more detail [13,14].)

For almost all of the results in Table 2, and all of the results in Table 3, the yields of the biologically active smoke constituents in the test and control cigarettes were either not statistically significantly different, or significantly lower in the test cigarette. The only instances where statistically significant increases were obtained with the test cigarette relative to the control, and remained significant within the long-term analytical variability, are:

test cigarette B5, propionaldehyde (12.1 μg or 22% increase);
test cigarette C3, furfural (2.5 μg or 56% increase);
test cigarette C9, furfural (2.0 μg or 46% increase);
test cigarette C9, *o*-cresol (0.6 μg or 15% increase).

The increased yield of propionaldehyde in test cigarette B5 is similar to the maximum increase predicted from the pyrolysis of carboxymethyl cellulose, indicating that contributions from the ingredient are possible. For the other three cases, the increases observed in smoke yields are substantially less than those predicted from pyrolysis. Thus, for these non-volatile ingredients the pyrolysis technique has over-predicted the amount of decomposition/oxidation of the ingredient, and the generation of 'Hoffmann analytes' that would occur in a burning cigarette.

The increases in biologically active smoke components are important in assessing the total toxicological impact of the ingredients and the reasons for the increases are considered further, as follows. Test cigarette C3 contained 10.5% added white sugar and 0.9% acetic acid and produced a 2.5 μg (56%) increase in furfural yield relative to its control cigarette (Table 2). On the other hand, a cigarette with 10.5% added white sugar and no other ingredients had a furfural yield that was not statistically different from its control cigarette (Table 3). A cigarette containing 6.2% brown sugar as a single ingredient gave a furfural smoke yield that was 15% lower than its control cigarette, with statistical significance (Table 3). The 2.5 μg (56%) increased yield of furfural with test cigarette C3 must be due to an interaction involving both sugar and acetic acid during pyrolysis. It is known that heating sugars above about 120 °C under mildly acidic conditions produces furfural [15]. This process is in fact used for the commercial production of furfural by the steam distillation of sugar cane bagasse (fibrous residue from sugar cane), corn cobs, oat hulls and other natural material containing pentose residues under acidic conditions [15,16]. It should be noted that the levels of both ingredients tested in cigarette C3 were substantially higher than the maximum levels used on cigarettes: white sugar was tested at 10.5% (typical maximum use level on British American Tobacco cigarettes is 2.5%); acetic acid was tested at 0.9% (typical maximum use level is 0.05%).

Test cigarette C9 had its smoke furfural yield increased by 2.0 μg (46%) relative to its control cigarette (Table 2).

Table 2
Effect of mixtures of ingredients on smoke yields for those ingredients that produce biologically active products during their pyrolysis

Ingredient[a] (maximum cigarette level[b], ppm)	Amount (ppm)[c]	Smoke constituent	Smoke yield (S.D.)[d] (μg/cigarette)	
			Test	Control
Added to test cig A2				
Vanilla oleoresin (326)	2460	Phenol	11.5 (0.51)[e]	13.8 (0.83)
Added to test cig A5				
Coriander seed oil (560)	795	Styrene	12.1 (0.49)	11.6 (0.75)
Styrax extract (resinoid) (30)	65			
Added to test cig A8				
Vanilla, absolute (326)	381	*m* + *p*-Cresol	9.3 (0.44)[e,f]	10.9 (0.67)
		o-Cresol	2.9 (0.12)[e,f]	3.5 (0.20)
Added to test cig B2				
Brandy, absolute (40)	47	2-Butanone	77.2 (3.2)	81.4 (2.5)
Celery seed oleoresin (10)	12	Furfural	6.23 (0.51)	5.00 (0.70)
Potassium citrate (10)	12	Benzene	63.5 (1.9)[e]	67.0 (1.2)
Prune juice concentrate (10,900)	20000	Toluene	129 (2.3)	135 (2.4)
Sodium benzoate (5)	12	Styrene	18.3 (1.0)[e]	20.0 (0.5)
Sugar, brown (56,000)	62000	Phenol	23.2 (1.7)[e]	26.3 (1.8)
Added to test cig B3				
Ammonium glycyrrhizinate (52)	100	2-Butanone	77.3 (3.6)	81.4 (2.5)
Apple extract (200)	234	Furfural	5.47 (0.40)	5.00 (0.70)
Caramel (500)	16000	Benzene	67.3 (1.6)	67.0 (1.2)
Carob bean extract (roasted) (3400)	7000	Toluene	134 (2.4)	135 (2.4)
Carob bean powder (7000)	7000	Styrene	18.8 (0.50)[e]	20.0 (0.51)
Catechu powder (1)	12	Pyridine	21.0 (1.0)	22.6 (1.3)
Cherry juice (10)	12	Phenol	24.8 (1.4)	26.3 (1.8)
Chocolate (2700)	7000	*m*+*p*-Cresol	16.1 (1.3)	17.6 (1.1)
Cocoa shell extract (12,000)	20000	*o*-Cresol	5.38 (0.23)	5.75 (0.31)
Dextrin (1)	12			
Fenugreek tincture (500)	585			
Guar gum (2)	100			
Honey, absolute (30)	35			
Pineapple extract (10)	12			
Pipsissewa leaves extract (10)	12			
Plum extract (40)	3500			
Potassium sorbate (500)	6000			
Sodium benzoate (5)	12			
Sodium citrate (5)	12			
Valerian root tincture (100)	234			
Added to test cig B4				
Cocoa powder (20,000)	37700	2-Butanone	72.5 (6.3)[e]	81.4 (2.5)
Licorice extract, powder (20,000)	20000	Furfural	5.70 (0.00)	5.00 (0.70)
		Toluene	131 (3.6)	135 (2.4)
		Styrene	19.1 (0.78)	20.0 (0.51)
		Pyridine	18.8 (1.6)[e]	22.6 (1.3)
		Phenol	19.8 (2.4)[e,f]	26.3 (1.8)
		m + *p*-Cresol	14.1 (1.3)[e,f]	17.6 (1.1)
		o-Cresol	4.29 (0.35)[e,f]	5.75 (0.31)
Added to test cig B5				
Acacia powder (15,000)	15000	2-Butanone	82.0 (4.8)	81.4 (2.5)
Carboxymethyl cellulose (1000)	1000	2-Butenal	35.2 (2.5)[e]	31.3 (1.5)
Cellulose fibre (17,000)	28400	Propionaldehyde	66.2 (4.1)[e,f]	54.1 (1.9)
Hydroxypropyl cellulose (3300)	4000	Furfural	6.27 (0.91)	5.00 (0.70)
Starch (19,000)	19000	Benzene	63.7 (1.1)	67.0 (1.5)
Xantham gum (3800)	5000	Toluene	124 (3.2)[e]	135 (2.4)
		Styrene	18.4 (0.70)[e]	20.0 (0.51)
		Phenol	17.3 (1.3)[e,f]	26.3 (1.8)
		m + *p*-Cresol	12.7 (0.55)[e,f]	17.6 (1.1)
		o-Cresol	4.04 (0.26)[e]	5.75 (0.31)
Added to test cig C2				
Cocoa powder (20,000)	37700	2-Butanone	82.2 (1.6)	78.0 (4.4)

Table 2 (*Continued*)

Ingredient[a] (maximum cigarette level[b], ppm)	Amount (ppm)[c]	Smoke constituent	Smoke yield (S.D.)[d] (μg/cigarette)	
			Test	Control
		Furfural	5.73 (0.29)[e]	4.43 (0.25)
		Toluene	110 (2.4)	1.07 (2.1)
		Styrene	13.9 (0.67)	13.5 (1.1)
		Phenol	17.6 (1.3)	17.8 (0.28)
		m + *p*-Cresol	12.4 (0.73)	12.1 (0.32)
		o-Cresol	4.14 (0.24)	4.14 (0.10)
Added to test cig C3				
Sugar, white (25,000)	105,000	Butanal	37.4 (2.3)	36.8 (2.4)
Acetic acid (500)	9000	2-Butanone	79.3 (3.9)	78.0 (4.4)
		Furfural	6.90 (0.95)[e,f]	4.43 (0.25)
		Benzene	55.0 (0.85)	56.0 (0.99)
		Toluene	103 (0.6)[e]	107 (2.1)
		Styrene	12.1 (0.92)	13.5 (1.1)
		Phenol	16.1 (0.62)[e]	17.8 (0.28)
		m + *p*-Cresol	12.2 (0.32)	12.1 (0.32)
		o-Cresol	4.20 (0.11)	4.14 (0.10)
Added to test cig C5				
Apricot extract (560)	600	Furfural	5.37 (0.47)[e]	4.43 (0.25)
Honey (34,000)	45400	Toluene	110 (3.2)	107 (2.1)
Orris root extract (40)	100	Styrene	13.7 (0.75)	13.5 (1.1)
Pectin (80)	300	Phenol	15.3 (1.4)[e]	17.8 (0.28)
Plum extract (40)	3500			
Sorbitol[g] (24,000)	35300			
Added to test cig C7				
Chocolate (2700)	7000	Furfural	5.23 (0.49)	4.43 (0.25)
Corn syrup (17,000)	62000	Benzene	54.2 (2.1)	56.0 (0.99)
		Toluene	105 (2.9)	107 (2.1)
		Pyridine	14.8 (0.94)	15.2 (0.41)
		Phenol	15.3 (0.82)[e]	17.8 (0.28)
		m + *p*-Cresol	11.7 (0.48)	12.1 (0.32)
		o-Cresol	3.99 (0.31)	4.14 (0.10)
Added to test cig C8				
Alfalfa extract (34)	100	2-Butanone	80.8 (4.6)	78.0 (4.4)
Carob bean extract (3400)	5000	2-Butenal	36.0 (0.68)	34.5 (2.5)
Coffee extract (100)	2700	Furfural	5.93 (0.64)[e]	4.43 (0.25)
Fenugreek extract (175)	200	Benzene	55.7 (1.8)	56.0 (1.0)
Fig extract (800)	11700	Toluene	108 (2.2)	107 (2.1)
Kola nut extract (40)	100	Styrene	13.4 (0.48)	13.5 (1.1)
Maple syrup (50)	100	Pyridine	14.7 (0.41)	15.2 (0.41)
Oak chip extract (1)	100	Phenol	15.5 (1.1)[e]	17.8 (0.28)
Raisin extract (10,000)	11400	*m* + *p*-Cresol	11.8 (0.66)	12.1 (0.32)
Valerian root extract (560)	600	*o*-Cresol	3.98 (0.35)	4.14 (0.10)
Added to test cig C9				
Licorice extract, powder (20,000)	20000	Furfural	6.47 (0.81)[e,f]	4.43 (0.25)
Sugar, invert (62,000)	70000	Pyridine	15.2 (0.63)	15.2 (0.41)
		Phenol	19.6 (0.88)[e]	17.8 (0.28)
		m + *p*-Cresol	13.7 (0.54)[e]	12.1 (0.32)
		o-Cresol	4.75 (0.20)[e,f]	4.14 (0.10)

[a] Several ingredients were added to each test cigarette. In general, only those ingredients listed in Table 1 are included here. Tobacco was a U.S. blended tobacco.

[b] Typical maximum-use level on British American Tobacco products.

[c] Amount added to test cigarette, parts per million on a dry-weight of tobacco basis.

[d] S.D. is standard deviation, five replicate determinations for all analytes except furfural, which was three replicate determinations.

[e] Significantly different from control value at 95% confidence level—this data set.

[f] Also significantly different from control value at 95% confidence level when long-term analytical method variability is included.

[g] Detailed results for the pyrolysis of sorbitol are given in Baker and Bishop [3].

Table 3
Effect of single ingredients on furfural smoke yields[a]

Ingredient (maximum cigarette level[b], ppm, %)	Amount (%)[c]	Furfural yield (S.D.)[d] (μg/cigarette)	
		Test	Control
Cellulose fibre (1.7)	2.4	7.7 (0.3)[e]	11.0 (0.4)
Glucose (6.2)	6.2	5.8 (0.6)	5.9 (0.2)
Sorbitol (2.4)	3.6	7.8 (0.7)	8.4 (0.9)
Sugar, brown (6.2)	6.2	9.4 (0.0)[e]	11.0 (0.4)
Sugar, white (6.2)	10.5	12.8 (0.5)	11.0 (0.4)
Sorbitol + sugar mixture	6.7	7.7 (1.9)	8.4 (0.9)

[a] Ingredient added to U.S. blended tobacco that did not contain any reconstituted sheet and was uncased. Furfural determined in whole smoke.
[b] Typical maximum-use level on British American Tobacco products.
[c] Amount added to tobacco on a dry-weight of tobacco basis.
[d] S.D. is standard deviation, two replicate determinations.
[e] Significantly different from control value at 95% confidence level—this data set.

The test cigarette C9 contained two ingredients that could potentially increase the smoke furfural yield: licorice extract powder and invert sugar (Table 2). Licorice extract powder has in fact been tested on two cigarettes B4 and C9. The smoke furfural yield with cigarette B4 is statistically the same as that of its control cigarette (Table 2). Furthermore, sugars added as single ingredients to tobacco do not, in general, increase the smoke yield of furfural (Table 3). Consequently, the increases in smoke furfural yield with test cigarette C9 must be due to an interaction involving both invert sugar and licorice during the pyrolysis.

The 0.6 μg (15%) increase in *o*-cresol yield in test cigarette C9 could have been due to generation from pyrolysis of ingredients. However, given the range of yields of this analyte across different unfiltered cigarettes (Table 1), we do not consider this increase important. It is worth noting that the test cigarette C9 contains two ingredients that could potentially increase the phenol and cresol smoke yields: licorice extract powder and invert sugar (Table 2). Licorice extract powder has in fact been tested on two cigarettes B4 and C9 [13,14]. The phenol and cresol smoke yields with cigarette B4 are actually lower than those of its control cigarette (Table 2). Consequently, the increases in smoke phenol and cresol yields with test cigarette C9 must be due to invert sugar.

4. Conclusions

(1) A pyrolysis technique has been used as a first step in the total toxicological assessment of 159 non-volatile tobacco ingredients. Fifty-six of the ingredients were predicted to be potentially capable of yielding products of toxicological concern in smoke. These ingredients have been further assessed by adding them to cigarettes, machine-smoking the cigarettes and comparing their yields to those from a control (no ingredient) cigarette. It was found that in general the ingredients added to cigarettes do not increase the smoke components relative to the control cigarette.
(2) The pyrolysis technique gives reasonable predictions for the behaviour of semi-volatile ingredients in a burning cigarette in terms of distillation versus pyrolytic decomposition. However, the technique tends to over-predict the amount of decomposition that non-volatile ingredients undergo relative to their behaviour in a burning cigarette. In some cases, large over-estimates of pyrolysis products are predicted, especially furfural from sugars. In other words, the pyrolysis technique can produce false positives, especially for non-volatile ingredients.
(3) Less severe decomposition of the non-volatile ingredients actually occurs in the burning cigarette relative to in the pyrolysis system. Those non-volatile ingredients that do not generate products of toxicological concern in the pyrolysis system are unlikely to do so in a burning cigarette.
(4) This general pyrolysis technique is thus a first step in the total toxicological assessment of tobacco ingredients and is a useful screening tool for indicating which ingredients may yield biologically active products during decomposition of the ingredients.
(5) Some relevant products, such as formaldehyde and carbon monoxide, are not detected by the gas chromatography–mass spectrometer system used in this study. The generation and detection of these products during the pyrolysis of selected tobacco ingredients is the subject of a parallel paper [17].

Appendix A

A.1. Pyrolytic behaviour of individual tobacco ingredients

CAS No. is Chemical Abstract Service Registry Number.

Max. cig. appln. level (ppm) is the maximum recommended level of this ingredient applied commercially to a cigarette by British American Tobacco.

Composition of pyrolysate refers to the five most abundant pyrolysis products detected, together with any 'Hoffmann analyte' or other biologically active substance detected as pyrolysis products. Water, CO, CO_2 and products with a molecular weight below about 40 are not detected.

Max. smoke (μg) is the maximum level in cigarette smoke obtained from the ingredient, calculated as indicated in the text and assuming that the extent of pyrolysis observed in this study occurs in a burning cigarette.

Compounds in bold are biologically active and many are 'Hoffmann analytes'.

Levels in italics are at or below the daily threshold level of 0.03 μg for one cigarette.

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
Acacia powder 9000-01-5	15000	Acetol	20.7	1550
		Acetic acid	7.5	560
		Xanthosine	5.0	380
		Benzenediol	4.7	380
		Furfural	3.2	240
		2-Butanone	0.5	38
Alfalfa extract 84082-36-0	34	Hydroxymethylfurfural	22.8	4
		Furfuryl alcohol	14.7	2.5
		Vinylmethoxyphenol	7.0	1
		Maltol + hydroxylmethylpyranone	5.2	0.9
		Phenol + acetylthiophene	3.2	0.5
		Furfural + ?	1.4	0.2
Ammonium glycyrrhizinate 53956-04-0 $C_{42}H_{62}O_{16}NH_45H_2O$	52	**Phenol**	8.6	2
		Formylpyrrole	7.4	2
		Cresol	3.8	1
		Dihydrobenzofuran	3.1	0.8
		Toluene	2.6	0.7
		Pyrrole	2.4	0.6
Amyris oil 8015-65-4	5	Valencene	37.9	0.9
		Selinadiene	10.9	0.3
		β-Maaliene	8.9	0.2
		β-Elemene + ?	7.9	0.2
		β-Selinene	6.9	0.2
Angelica root oil 8015-64-3	2.5	Phellandrene	19.9	0.2
		α-Pinene	16.7	0.2
		δ-Carene	14.6	0.2
		Sabinene	5.9	0.07
		β-Myrcene	3.8	0.05
Angelica root tincture/extract 84775-41-7	105	No products detected	–	–
Apple extract 85251-63-4	200	Hydroxymethylfurfural	81.0	80
		Furfural	5.5	6
		Methylfurural	1.6	2
		Methylbenzenediol?	1.2	1
		Dimethylfurfural?	1.1	1
Apricot extract 68650-44-2 Diluted with glycerol	560	Glycerol	68.4	190
		Hydroxymethylfurfural	23.7	66
		γ-Undealactone	2.1	6
		Furfural	1.5	4
		Vanillin	1.4	4
Balsam oil, Peru 8007-00-9	56	Benzyl benzoate	58.1	16
		Benzyl cinnamate	36.1	10
		Benzoic acid	1.5	0.4
		Cinnamic acid	0.7	0.2
		Vanillin	0.6	0.2
Benzoin absolute, Sumatra 84012-39-5	0.5	Cinnamic acid	50.4	0.1
		Benzoic acid	10.5	*0.03*
		Cinnamyl cinnamate	3.5	*0.009*
		Benzyl cinnamate	3.0	*0.008*
		Benzyl benzoate	2.2	*0.006*
		Phenol	1.2	*0.003*
		Cresol + ?	0.3	*0.001*

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
Black currant buds, absolute 68606-81-5	5	Dehydroisolongifolone	14.0	0.4
		Caryophyllene	11.3	0.3
		Aminobenzamide	11.3	0.3
		Unidentified product	8.9	0.2
		Dibenzobenzonitrile	5.6	0.1
Bois de rose oil 8015-77-8	1	Linalool	81.7	0.4
		Linalool oxide	10.4	0.05
		Limonene + cineole	3.8	*0.02*
		Methyl heptenone	0.8	*0.004*
		Linalyl oxide	0.7	*0.004*
Brandy, absolute	40	Methyl butanol	73.6	15
		Isoamyl alcohol	10.3	2
		Methylpropanol	4.0	0.8
		Isoamyl acetate	0.9	0.2
		Ethyl octanoate	0.8	0.2
		Furfural	0.2	0.04
Buchu leaf oil 68650-46-4	2.5	Limonene	31.8	0.4
		Menthone	21.2	0.3
		Pulegone	11.5	0.1
		Isomenthone	8.5	0.1
		Buchu camphor	7.8	0.1
Calcium carbonate 471-34-1 $CaCO_3$	9000	No products detected	–	–
Cananga oil 68606-83-7	2.5	Linalool	24.1	0.3
		α-Gurjunene	19.6	0.2
		Caryophyllene	11.7	0.1
		Amyl cinnamic aldehyde	10.0	0.1
		Anethole	3.8	0.05
		Cresol	0.6	*0.008*
Caramel 8028-89-5	500	Acetic acid	42.7	110
		Theobromine	25.6	64
		Long chain hydrocarbons	12.2	31
		Methylfurfural	6.6	17
		Acetylfuran	3.2	8
		Furfural	2.5	6
Caraway seed oil 8000-42-8	2.5	Limonene	51.1	0.6
		Carvone	45.2	0.6
		Dihydocarvone	1.3	*0.03*
		β-Myrcene	0.4	*0.005*
		Neohydrocarveol	0.3	*0.004*
Carboxymethyl cellulose 9000-11-7	1000	Acetol	13.1	66
		Unidentified product	5.9	30
		Dimethylcyclopentenolone	4.1	21
		Acetic acid	3.7	19
		Cresol + ?	3.4	17
		Methylhydroquinone	2.9	15
		Propionaldehyde	2.6	13
		Phenol	1.5	8
		Furfural	1.1	6
		Toluene	0.7	4
Cardamon seed oil 8000-66-6	76	α-Terpinolene	37.5	14
		Cineole	26.5	10
		γ-Terpinene + linalyl acetate	4.4	2
		Linalool	3.4	1
		Sabinene	2.6	1
Carob bean extract 84961-45-5	3400	Propylene glycol	65.3	1100
Diluted with propylene glycol		Acetic acid	24.5	420

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Acetol	3.4	58
		Furfural	1.5	26
		Pyruvaldehyde	1.0	17
Carob bean extract (roasted) 84961-45-5 Diluted with glycerol	3400	Glycerol	94.1	1600
		Acetic acid	1.3	22
		Acetol	1.0	17
		Methyl oleate	0.4	7
		Furfural	0.3	5
Carob bean powder 9000-40-2	7000	Acetic acid	23.5	820
		Hydroxymethylfurfural	13.3	470
		Furfural	8.1	280
		Benzoic acid	7.3	260
		Acetol	6.3	220
Carob bean tincture 84961-45-5 Diluted with ethanol and water	700	No products detected	–	–
Cascarilla bark oil 8007-06-5	10	Cymene	13.1	0.7
		α-Gurjunene + caryophyllene	11.3	0.6
		α-Humulene	5.7	0.3
		α-Calacorene	3.3	0.2
		Cuparene	1.9	0.1
Cassia bark oil 8007-80-5	30	Cinnamaldehyde	76.2	11
		Methoxy cinnamyl aldehyde	13.1	2
		Cinnamyl acetate	4.1	0.6
		Coumarin	1.8	0.3
		Anisaldehyde	0.7	0.1
Cassia, absolute 89958-31-6	0.5	Ethyl linoleate	15.9	0.04
		Nonadecane	14.4	0.04
		Acetic anhydride?	9.3	*0.02*
		Methyl anisate	7.2	*0.02*
		Trimethylpentadecanone	6.6	*0.02*
Catechu powder 8007-76-1	1	Pyrocatechol	31.6	0.2
		Acetol	11.6	0.06
		Acetic acid	11.4	0.06
		Phenol	11.1	0.06
		Cresol	5.2	*0.03*
		Pyridine	0.8	*0.004*
		Furfural	0.2	*0.001*
Celery seed oil 8015-90-5	10	Limonene	57.1	3
		β-Selinine	16.4	0.8
		Ledol	6.5	0.3
		α-Selinine	5.8	0.3
		Butylphthalide	4.3	0.2
Celery seed oleoresin 8015-90-5	10	Propenylphenoxyacetate + dihydrobutylphthalate	37.0	2
		Butylphthalate?	15.9	0.8
		Limonene	13.9	0.7
		β-Selinine	5.2	0.3
		Acetic acid	3.6	0.2
		Styrene	2.8	0.1
Cellulose fibre 65996-61-4	17000	Hydroxymethylfurfural	9.9	840
		Acetol	7.6	650
		Methyl formate? and/or hydroxyacetaldehyde	6.3	540
		Furfural	4.8	410
		Methyl pyruvate	4.3	370
		Benzene	3.1	260
		Acetic acid + **2-butenal**	2.6	220
		Phenol + methylfuranone + ethyltoluene	2.1	180

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Toluene	1.0	85
		Cresol	0.9	77
		Styrene	0.7	60
Chamomile extract, Roman 8015-92-7	530	Isobutyl angelate	36.4	96
		Methylbutyl angelate	25.2	67
		n-Butyl angelate	8.7	23
		Butyl isobutyrate	4.7	12
		Isopentyl isobutanoate	3.2	8
Chamomile oil, Hungarian 8002-66-2	75	Bisabolol oxide	59.9	22
		β-Farnesene	11.1	4
		Bisabolone oxide	5.8	2
		En-in-dicycloether?	4.7	2
		Chamazulene	4.0	1.5
Chamomile oil, Roman 8015-92-7	78	Isobutyl angelate	36.5	14
		Methylbutyl angelate	21.9	9
		Unidentified compound	7.9	3
		Carenol and/or pineol	3.5	1
		Pinocarvone	2.1	0.8
Cherry juice 89997-53-5	10	Hydroxymethylfurfural + ?	54.1	2.7
		Acetic acid	16.1	0.8
		Acetic anhydride	12.0	0.6
		Furfural	6.5	0.3
		Methylpyrazinylmethanol?	2.6	0.1
Chocolate	2700	Palmitic acid	11.9	160
		Heptadecene	7.0	95
		Stearic acid	5.7	77
		Pentadecene	4.8	65
		Oleic acid	3.9	53
		Caffeine	1.5	20
		Phenol	1.1	15
		Toluene	0.9	12
		Benzene	0.5	7
		Cresol + ?	0.5	7
		Pyridine	0.5	7
		Furfural + methylfuran	0.4	5
Cinnamon bark oil 8015-91-6	30	Cinnamaldehyde	69.1	10
		Isoeugenol	10.7	2
		Linalool	6.1	0.9
		β-Phellandrene + limonene	2.5	0.4
		β-Caryophyllene	2.2	0.3
Citronella oil 8000-29-1	2	Geraniol	19.7	0.2
		Methyl isoeugenol	19.1	0.2
		Limonene	6.0	0.06
		Borneol	5.7	0.06
		Dimethylmethylpentylbicycloheptene + α-bergamotene	3.7	0.06
Clary sage infusion 84775-83-7	10	Benzyl alcohol	92.7	5
		Benzaldehyde	6.7	0.3
		δ-Carene	0.6	*0.03*
Clary sage oil 8016-63-5	10	δ-Carene	68.5	3
		β-Myrcene	5.8	0.3
		Carene (unspecified)	5.2	0.3
		β-Ocimene	3.5	0.2
		α-Terpineol	2.2	0.1
Cocoa distillate 84649-99-2	100	No products detected	–	–
Cocoa extract 84649-99-3	20000	Propylene glycol	67.2	6700
Diluted with propylene glycol		Glycerol	26.9	2700

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Acetic acid	3.0	300
		Methylbutanal	0.7	70
		Isobutanal	0.4	40
Cocoa powder 84649-99-0	20000	Acetic acid	27.2	2,700
		Acetol	6.6	660
		Furfuryl alcohol	6.6	660
		Caffeine	4.0	400
		Pyrrole	2.8	280
		Furfural + cyclopentanone	2.1	210
		Phenol	1.6	160
		Cresol + pyridenediol	1.4	140
		2-Butanone	0.9	90
		Toluene	0.7	70
		Styrene	0.2	20
Cocoa shell extract 8002-31-2	12000	Methyl octadecenoate	12.2	730
		Methyl palmitate	11.9	710
		Oleic acid	10.5	630
		Palmitic acid	7.6	460
		Methyl stearate	6.9	410
		Cresol	0.2	12
		Phenol	0.2	12
		Furfural	0.1	6
		Styrene	0.1	6
Coffee extract 93348-12-0	100	Caffeine	25.9	13
		Palmitic acid	13.8	7
		Acetic acid	12.2	6
		Ethyl palmitate	5.2	3
		Acetal + ?	4.9	2
		Pyridine	3.7	2
		Phenol	1.5	0.8
		Furfural + methylfuran	0.7	0.4
		Cresol	0.5	0.3
		Toluene	0.5	0.3
Cognac oil, green 8016-21-5	10	Ethyl caproate	39.2	2
		Ethyl laurate	29.3	1
		Ethyl palmitate	10.2	0.5
		Ethyl myristate	6.0	0.3
		Ethyl octanoate and/or ethyl caprylate	5.2	0.3
Cognac oil, white 977050-49-9	7.5	Ethyl decanoate	38.4	1
		Ethyl laurate	29.4	1
		Ethyl palmitate	14.8	0.6
		Ethyl myristate	5.1	0.2
		Ethyl octanoate	4.8	0.2
Coriander seed oil 8008-52-4	560	Linalool	72.5	200
		Camphor	7.1	20
		Cymene	5.0	14
		γ-Terpinene	2.8	8
		α-Pinene	2.7	8
		Styrene	0.1	0.3
Corn syrup 68131-37-3	17000	**Furfural**	45.3	3850
		Hydroxymethylfurfural	44.0	3850
		Methyl benzenediol	1.6	140
		Dihydrodihydroxymethylpyranone	1.2	100
		Furfuryl alcohol	0.7	60
		Phenol	0.4	30
Cumin seed oil 8014-13-9	2.5	Isopropylbenzaldehyde	27.5	0.3
		γ-Terpinene	17.3	0.2

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		β-Pinene	12.0	0.2
		Limonene	9.7	0.1
		Cymene	6.7	0.08
Davana oil 8016-03-3	10	Davanone	56.8	3
		Ethyl cinnamate	8.2	0.4
		γ-Muurolene and/or β-cubebene	4.1	0.2
		Germacrene	3.4	0.2
		β-Selinene	3.0	0.2
Dextrin 9004-53-9	1	Hydroxymethylfurfural	50.1	0.3
		Furfural	23.5	0.1
		Unidentified compound	4.8	*0.02*
		Furfuryl alcohol?	4.2	*0.02*
		Methyl resorcinol	1.8	*0.009*
Diammonium hydrogen phosphate 7783-28-0 $(NH_4)_2HPO_4$	10000	No products detected	–	–
Dill herb oil 8006-75-5	10	Carvone	43.8	2
		Limonene	30.9	2
		Phellandrene	10.1	0.5
		Dill ether	4.4	0.2
		Dihydrocarvone	2.3	0.1
Dill seed oil 8016-06-6	1	Carvone	79.5	0.4
		Limonene	14.3	0.07
		Dihydrocarvone	5.0	*0.03*
		Methylenecyclononene?	0.3	*0.002*
		Menthatriene	0.1	*0.001*
Fenugreek extract 84625-40-1	175	Ethyl linoleate	37.4	33
		Ethyl palmitate	14.8	13
		Ethyl stearate	10.6	9
		Palmitic acid	6.0	5
		Hydroxydimethylfuranone	3.4	3
		Pyridine	0.4	0.4
		2-Butanone	0.3	0.3
		Benzene + methylbutenal	0.2	0.2
		Toluene + pentanol	0.2	0.2
		2-Butenal? + ?	0.1	0.09
		Furfural	0.1	0.09
Fenugreek oil 84265-40-1	5	Diethyl tartrate	74.3	2
		Acetic anhydride	4.7	0.1
		Acetic acid	4.7	0.1
		Ethyl oleate	3.9	0.1
		Ethyl linoleate	2.4	0.06
Fenugreek tincture 84265-40-1	500	Heptanoic acid	71.4	180
		Acetic acid	5.2	13
		Pyridine	3.4	9
		Vinylphenol	2.5	6
		Phenol	2.3	6
		Furfural	0.5	1
Fig extract 68916-52-9	800	Acetic acid	45.1	180
		Furfural	24.5	98
		Sorbic acid	10.2	41
		Unidentified compound	8.6	34
		Butanediol	3.7	15
d-Fructose 57-48-7	2100	Hydroxymethylfurfural	71.1	750
		Furfural	7.9	80
		Dihydrodihydroxymethyl pyranone	2.9	30
		Acetic acid	1.3	14

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Methylfurfural	1.2	13
Galbanum extract (resinoid) 9000-24-2	1	α- and/or β-Pinene	21.4	0.1
		Valencene	6.6	*0.03*
		Unidentified compound	5.7	*0.03*
		Hydroxycoumarin	4.9	*0.03*
		α-Amorphene and/or α-muurolene	4.3	0.02
Galbanum oil 8023-91-4	2	β-Pinene	48.6	0.5
		γ-Carene	14.5	0.1
		α-Pinene	8.4	0.08
		β-Phellandrene + limonene	3.6	0.04
		Cymene	3.1	*0.03*
Geranium oil 8000-46-2	30	β-Citronellol	31.1	5
		Nerol	12.9	2
		Citronellyl acetate and/or formate	7.8	1
		α-Gurjunene and/or maaliene	7.6	1
		Menthone	5.1	0.8
Ginger oil 8007-08-7	57	α-Zingiberene	28.0	8
		β-Sesquiphellandrene	15.6	4
		α-Curcumene	12.0	3
		β-Bisabolene	9.1	3
		α-Farnesene	6.1	2
Ginger oleoresin 84696-15-1	15	α-Zingiberene	29.0	2
		β-Sesquiphellandrene	13.7	1
		α-Curcumene	8.8	0.7
		Unidentified compound	8.0	0.6
		Zingerone	6.2	0.5
Glucose 9055-00-9	1300	Hydroxymethylfurfural	50.0	325
		Furfural	5.4	35
		Acetic acid + hydroxyacetaldehyde?	3.8	25
		Dihydroxymethyl pyranone	3.6	23
		Methylbenzenediol	3.0	20
Grapefruit oil, expressed 8016-20-4	2.5	Limonene	96.6	1
		β-Myrcene	1.4	*0.02*
		α-Pinene	0.4	*0.005*
		Decanal	0.3	*0.004*
		Caryophyllene	0.2	*0.003*
Grapefruit oil, terpeneless 90045-43-5	1	Limonene	71.0	0.4
		Caryophyllene	3.8	*0.02*
		Decanal	3.5	*0.02*
		Nookatone	3.0	*0.02*
		Octanal	2.8	*0.01*
Guaiac wood oil 8016-23-7	1	α-Patchouline	37.8	0.2
		Calarene	28.7	0.1
		β-Selinene	9.1	0.05
		δ-Selinene	4.6	*0.02*
		α-Gurjunene	3.3	*0.02*
Guar gum 9000-30-0	2	Hydroxymethylfurfural	13.4	0.1
		Acetol	11.9	0.1
		Acetic acid	9.9	0.1
		Methyl pyruvate	6.1	0.06
		Furfural	6.0	0.06
		Cresol	0.9	*0.009*
		Benzene	0.7	*0.007*
		2-Butanone	0.7	*0.007*
		Toluene	0.5	*0.005*
		Butenal	0.2	*0.002*

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
Honey 8028-66-8	34000	Hydroxymethylfurfural + ?	28.7	4,900
		Furfural	24.3	4,100
		Acetic acid	6.3	1,100
		Methylfurfural	5.6	950
		Methylbenzenediol	4.1	700
		Toluene	0.4	68
		Styrene + ?	0.2	34
Honey, absolute 91052-92-5	30	Hydroxymethylfurfural	19.4	3
		Acetic acid	18.3	3
		Sucrose?	15.7	2
		Furfural	13.1	2
		Dihydroxyacetone	11.5	2
Hydroxypropyl cellulose 9004-64-2	3300	Propylene glycol trimer	40.9	670
		Hydroxypropoxypropanol	21.1	350
		Propylene glycol	10.9	180
		Unidentified compound	5.6	92
		Acetol	4.7	78
		Furfural + ?	0.5	8
		Phenol + ?	0.5	8
Immortelle, absolute 8023-95-8	0.5	9 Unidentified compounds	48.5	0.1
		γ-Terpinene and/or neryl acetate	3.4	*0.009*
		Ethyl palmitate	3.3	*0.008*
		α-Curcumene	3.3	*0.008*
		Ethylmethylbutanoate	3.3	*0.008*
		Acetaldehyde?	0.6	*0.002*
Jasmin, absolute 8031-01-4	5	Neophytadiene	11.3	0.3
		Benzyl benzoate	10.7	0.3
		Benzyl acetate	9.6	0.2
		Methyl linolenate + heneicosane	5.3	0.1
		Methyl palmitate	2.6	0.07
		Cresol	0.6	*0.02*
Jasmin oil 8022-96-6	2.5	Benzyl acetate	26.1	0.3
		Benzyl benzoate	25.3	0.3
		Linalool	7.5	0.09
		Neophytadiene	7.1	0.09
		Benzenemethanol	4.2	0.05
		Cresol	1.1	*0.01*
Kola nut extract 68916-19-8 Diluted with glycerol and propylene glycol	40	Propylene glycol	72.6	15
		Glycerol	18.0	4
		Vanillin	0.7	0.1
		Acetic acid	0.6	0.1
		Hydroxymethylfurfural	0.5	0.1
		Furfural	0.4	0.08
Kola nut tinctute 68916-19-8	370	1 Unidentified compound	98.5	180
		3 Unidentified compounds	1.5	19
Labdanum, absolute 68917-77-1	15	1 Unidentified compound	36.8	3
		Aromadendrene and/or gurunene	12.9	1
		Acetamide	10.5	0.8
		Trimethylnaphthalene?	5.3	0.4
		Pentylfuran?	3.3	0.2
Labdanum oil 8016-26-0	1	α-Pinene	10.9	0.06
		Ledene	10.8	0.05
		Valencene	4.0	*0.02*
		Cymene	3.9	*0.02*
		Pinocarveol	3.7	*0.02*
Labdanum oleoresin 977092-72-0	2.5	Methyl ionone	23.4	0.3

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Unidentified compound	20.9	0.3
		Ethyl hydrocinnamate and/or ethylphenylpropionate	16.2	0.2
		Ethyl heptadecanoate	12.2	0.2
		Hydrocinnamic acid and/or phenylpropionic acid	7.7	0.1
		Acetaldehyde?	0.7	*0.009*
		Phenol	0.7	*0.009*
Lavender oil 8000-28-0	2.5	Linalool	27.7	0.3
		Cyclofenchene and/or linalyl acetate	23.2	0.3
		β-Myrcene	5.0	0.06
		Caryophyllene + α-santalene	4.6	0.06
		Lavandulyl acetate	4.4	0.06
Lemon extract 84929-31-7	10	Limonene	59.8	3
		β-Pinene and/or δ-carene	14.0	0.7
		γ-Terpinene	12.1	0.6
		α-Pinene	2.3	0.1
		β-Myrcene	2.0	0.1
Lemon oil, expressed 8020-19-7	10	Limonene	59.8	3
		β-Myrcene and/or β-Pinene	14.0	0.7
		γ-Terpinene	12.1	0.6
		α -Pinene	2.4	0.1
		α-Terpinolene	0.5	*0.03*
Lemon oil, terpeneless 68648-39-5	10	E-Citral	30.6	2
		Z-Citral	17.1	0.9
		Geranyl acetate	11.2	0.6
		Geranyl isobutyrate	7.0	0.4
		Limonene	5.0	0.3
Lemongrass oil 8007-02-1	2.5	E-Citral	47.3	0.6
		Z-Citral	31.1	0.4
		β-Geraniol	5.3	0.07
		β-Pinene and/or β-myrcene	3.6	0.05
		β-Caryophyllene	2.0	*0.03*
Licorice extract, powder 68916-91-6	20000	Acetic acid	42.0	4,200
		Acetol	11.9	1,200
		Furfuryl alcohol	11.7	1,200
		Diacetyl	4.1	410
		Acetol acetate	2.0	200
		Phenol	1.4	140
		Cresol	0.2	20
		Pyridine + pyrrole?	0.2	20
		Furfural	0.2	20
Lime oil, expressed 8008-26-2	10	Limonene	48.4	2
		γ-Terpinene	13.4	0.7
		β-Pinene	9.5	0.5
		E-Citral	2.7	0.1
		Cymene	2.3	0.1
Lovage oil 8016-31-7	7.5	Butylphthalide	74.6	3
		Butylidenephthalide	6.9	0.3
		Isobutylidenephthalide	3.8	0.1
		Sabinene + limonene	1.3	0.05
		Valerophenone and/or phenylpentanone	0.7	*0.03*
Mace oil 8007-12-3	10	Myristicin	22.2	1
		Sabinene	15.1	0.8
		α-Pinene	14.2	0.7
		β-Pinene	10.3	0.5
		Terpineol	6.0	0.3

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
Mandarin oil 8008-31-9	40	Limonene	60.4	12
		γ-Terpinene	20.5	4
		Cymene	3.6	0.2
		α-Pinene	1.8	0.09
		β-Myrcene	1.2	0.06
Maple, mountain maple solid extract 91770-22-8 Diluted with propylene glycol	20	Propylene glycol	91.9	9
		Acetic acid	1.5	0.2
		Acetol	1.4	0.1
		Acetoxypropanol	1.1	0.1
		Methylfurfural	0.6	0.06
Maple syrup 91770-22-8	50	Hydroxymethylfurfural	28.2	7
		Cytidine	18.2	5
		Acetic acid? + propanol?	18.1	5
		Furfural + ethanol?	15.1	4
		Dihydroxyacetone	3.8	1
Mate extract 68916-96-1 Diluted with propylene glycol	5	Propylene glycol	78.8	2
		Caffeine	9.2	0.2
		Acetic acid	3.2	0.08
		Acetol	2.2	0.06
		Pyruvaldehyde	1.5	0.04
		Furfural	0.3	*0.008*
		Phenol	0.1	*0.003*
Mimosa, absolute 93685-96-2	1	Heptadecene	20.8	0.1
		Nonadecane	18.3	0.09
		Ethyl palmitate	15.7	0.08
		Ethyl linolenate	8.2	0.04
		Palmitic acid	7.3	0.04
Molasses, sugar cane 68476-78-8	14000	Acetic acid	83.4	5,800
		Vinyl acetate?	16.6	1,200
Myrrh oil 8016-37-3	10	Unidentified compound	25.5	1
		Dimethyl(methylethenyl)ethenyldihrobenzofuran	17.9	0.9
		Unidentified compound	9.4	0.5
		β-Elemene	3.5	0.2
		Cardinol and/or β-cubebene	2.2	0.1
Neroli bigarde oil 8016-38-4	5	Linalool	40.1	1
		β-Myrcene and/or linalyl acetate	26.7	0.7
		α-Terpineol	4.7	0.1
		Limonene	4.1	0.1
		Lavandulyl acetate and/or geranyl acetate	3.6	0.09
Nutmeg oil 8008-45-5	10	Myristicin	16.3	0.8
		Sabinene	16.2	0.8
		α-Pinene	14.7	0.7
		β-Pinene	10.0	0.5
		Limonene + β-phellandrene	4.9	0.2
Oak chip extract 68917-11-3 Diluted with propylene glycol and glycerol	1	Propylene glycol	67.5	0.3
		Glycerol	26.8	0.1
		Acetic acid	0.5	0.3
		Furfural	0.5	0.3
		Acetol	0.2	0.1
		Benzene	0.05	*0.03*
Oakmoss, absolute 9005-5-4	5	Benzyl benzoate	20.6	0.5
		Methylresorcinol	20.6	0.5
		Methydimethylresorcylate	18.4	0.5
		Unidentified compound	15.8	0.4
		Ethyl oleate	6.9	0.2
Olibanum oil 8016-36-2	2.5	α-Pinene	34.6	0.4

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Limonene	15.0	0.2
		Caryophyllene	4.8	0.06
		Sabinene	4.6	0.06
		β-Myrcene	3.7	0.05
Opoponax oil 8021-36-1	1	Santalene	25.6	0.1
		α-Bisabolene	21.8	0.1
		Ocimene	16.1	0.08
		α-Bergamotene + dimethyl(methylpentenyl)bicycloheptene?	7.1	0.04
		β-Bisabolene	4.1	*0.021*
Orange flower, absolute 8016-38-4	0.05	Linalool	37.2	*0.009*
		δ-Carene	12.6	*0.003*
		Nerolidol	9.7	*0.002*
		Farnesol	8.5	*0.002*
		Indole	5.9	*0.002*
Orange juice essence oil 68606-94-0	100	Limonene	42.4	21
		Acetic acid	33.8	17
		Acetic anhydride	23.8	12
Orange leaf, absolute 977091-84-1	0.5	Linalool	41.0	0.1
		α-Terpineol	34.0	0.09
		β-Geraniol	12.1	*0.03*
		Nerol?	4.0	*0.01*
		Vinylmethoxyphenol	1.4	*0.004*
Orange oil, bitter 68916-04-1	1	Limonene	96.6	0.5
		β-Myrcene	1.4	*0.007*
		β-Pinene	0.5	*0.003*
		α-Pinene	0.4	*0.002*
		α-Terpinolene	0.4	*0.002*
Orange oil, sweet 8005-57-9	100	Limonene	97.0	49
		β-Myrcene	1.4	0.7
		δ-Carene	0.4	0.2
		α-Pinene	0.4	0.2
		Sabinene	0.3	0.2
Orange oil, sweet, terpeneless 68606-94-0	100	Limonene	44.6	22
		Decanal	9.5	5
		Linalool	5.8	3
		Calarene and/or valencene	3.6	2
		E-Citral	3.4	2
Orris root extract 8002-73-1	40	Ethyl myristate	34.2	7
		Myristic acid	15.6	3
		Acetic acid	14.3	3
		Unidentified compound	9.4	2
		Irone	6.1	1
		Phenol?	1.2	0.2
Palmarosa oil 8014-19-5	2.5	Geraniol	63.1	0.8
		Lavandulyl acetate	9.2	0.1
		E-Citral	8.0	0.1
		Linalool	4.9	0.06
		Ocimene	4.9	0.06
Patchouli oil 8014-09-3	10	Patchouli alcohol	41.0	2
		δ-Guaiene	12.4	0.6
		α-Guaiene	9.7	0.5
		Seychellene	8.0	0.4
		α-Patchoulene	5.2	0.3
Pectin 9000-69-5	80	**Furfural**	19.9	8
		Acetic acid	8.6	3

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Hydroxymethylfurfural + ?	5.6	2
		Methyl pyruvate	4.0	2
		Dimethyl succinate and/or dimethyl ester of oxo-pentanedioic acid	3.1	1
Pepper oil, black 8006-82-4	0.5	Caryophyllene	23.5	0.06
		Limonene	15.5	0.04
		β-Pinene	8.6	*0.02*
		Sabinene	7.4	*0.02*
		α-Pinene	5.1	*0.01*
Peppermint oil 8006-90-4	35	Menthol	44.9	8
		Menthone	19.9	3
		Menthofuran	10.4	2
		Menthol acetate	5.8	1
		Cineole	4.6	0.8
Peppermint oil, terpeneless 68606-97-3	100	Menthol	54.5	27
		Menthone	19.4	10
		Epoxymenthadiene?	9.0	5
		Menthol acetate	6.4	3
		Pulegone	2.0	1
Petitgrain oil, terpeneless	0.5	Cyclofenchene and/or vetiverol	39.7	0.1
		Linalool	26.0	0.07
		α-Terpineole	7.4	*0.02*
		Lavandulyl acetate	5.9	*0.02*
		β-Myrcene	3.8	*0.01*
Pineapple extract 97676-27-2	10	**Furfural**	44.6	2
		Acetic acid	19.0	1
		Unidentified product	19.0	1
		Ethyl phthalate	12.7	0.6
		Butanedione?	4.7	0.2
Pine needle oil 8021-29-2	0.5	Bornyl acetate	41.9	0.1
		Camphene	18.0	0.05
		α-Pinene	11.6	*0.03*
		Carene	11.0	*0.03*
		Limonene + sabinene and/or phellandrene	7.5	*0.02*
Pipsissewa leaves extract 89997-56-8 Diluted with propylene glycol	10	Propylene glycol	49.8	2
		Methylbenzenediol	11.3	0.6
		Hydroxymethylfurfural	8.0	0.4
		Furfural	5.4	0.3
		Acetol	3.0	0.2
Plum extract 90082-87-4 Diluted with propylene glycol and glycerol	40	Propylene glycol	61.9	12
		Hydroxymethylfurfurole	8.7	2
		Glycerol	7.9	2
		Ethylmethyldioxolane?	6.2	1
		Dihydrodihydroxymethylpyranone?	3.2	0.6
		Furfural	0.4	0.08
		Styrene + acetoxypropanol?	0.4	0.08
		Phenol	0.06	*0.01*
		Benzofuran	0.04	*0.008*
Potassium citrate 866-84-2	10	**Benzene**	8.3	0.4
		Pentylbenzene?	8.2	0.4
		Toluene	7.2	0.4
		Xylene	5.5	0.3
		2-Butanone	4.5	0.2
		Styrene	0.5	*0.03*
		Cresol	0.5	*0.03*
Potassium sorbate 24634-61-5	500	Propyltoluene	10.4	26

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Xylene	6.6	17
		Toluene	5.3	13
		Methylstyrene	5.0	13
		Benzene	3.2	8
		Styrene	1.9	5
		Phenol	0.9	2
		2-Butanone	0.1	0.3
Prune extract 90082-87-4 Diluted with propylene glycol	10900	Propylene glycol	95.1	5,200
		Glycerol	1.5	82
		Methoxyethanol	1.5	82
		Acetol	0.9	49
		Acetic acid	0.4	22
Prune juice concentrate 85594-37-2	10900	Hydroxymethylfurfural	79.9	4,400
		Acetic acid	5.3	290
		Furfural	4.9	270
		Propylhydroxy benzoate	2.0	110
		Methylbenzenediol	1.4	76
Raisin extract 68915-86-6	10000	Hydroxymethylfurfural	22.8	1,100
		Furfural	12.4	620
		Benzene? and/or isovaleraldehyde	12.0	600
		Acetic acid	5.3	270
		Toluene	3.4	170
		Phenol + cyclohexenone?	2.0	100
		Styrene	1.6	80
		Benzofuran	0.5	25
		Cresol	0.5	25
		2-Butanone	0.4	20
		Pyridine	0.2	10
		2-Butenal	0.1	5
Raspberry distillate 84929-76-0	1	Hydroxymethylfurfural? + methoxymethylpyrazine?	62.2	0.3
		Methylmaleic anhydride	25.2	0.1
		Furfural	5.7	*0.03*
		Dimethylfurfural	4.1	*0.02*
		Methylfurfural	2.8	*0.01*
Rose, absolute, red 90106-38-0	0.5	Benzene ethanol	53.8	0.1
		Nonadecane	13.5	*0.03*
		Heneicosane	8.8	*0.02*
		β-Citronellol	6.7	*0.02*
		Geraniol	2.7	*0.007*
Rose oil, red 90106-38-0	10	β-Citronellol	34.2	2
		Geraniol	18.6	0.9
		Nonadecane	8.8	0.4
		Phenethyl benzoate	4.2	0.2
		Heptadecane	2.5	0.1
Rosemary oil 8000-25-7	0.5	Cineole	22.2	0.06
		Camphor	21.0	0.05
		α-Pinene	20.5	0.05
		Camphene	10.5	*0.03*
		β-Pinene	4.7	*0.01*
Rum, dark 91450-09-8	250	Methylbutanol	47.5	59
		Hydroxymethylfurfural	10.5	13
		Acetic acid	9.5	12
		Formic acid + ?	9.5	12
		Dihydrodihydroxymethyl pyranone	5.2	7
Rum extract 90604-30-1	10	Ethyl myristate	15.4	0.8
		Ethyl laurate	15.2	0.8

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Methyl butanol and/or isoamyl alcohol	13.2	0.7
		Ethyl decanoate	7.9	0.4
		Unidentified compound	6.3	0.3
		Cresol + methoxyethoxyethylfuran?	0.6	*0.03*
		Furfural	0.1	*0.005*
Rum, white 90604-31-1	250	Acetic acid	32.5	41
		Acetic anhydride?	30.1	38
		Isobutanol	9.0	11
		Ethyl acetate	8.2	10
		Methylbutanol	6.8	9
Sage oil 8022-56-8	7.5	Thujone	26.5	1
		Camphor	19.8	0.7
		Eucalyptol	8.8	0.3
		β-Caryophyllene	6.0	0.2
		Borneol	5.3	0.2
Sandalwood oil, yellow 8006-87-9	7.5	α-Santalol	44.3	2
		β-Santalol	23.9	0.9
		Cymene	7.1	0.3
		Epi-Santalol	3.8	0.1
		Curcumene?	2.7	0.1
Sodium acetate 127-09-3	10	3 Long chain hydrocarbons	55.9	3
		Pentacosane	17.2	0.9
		Tetracosane	7.7	0.4
		Acetic acid	6.1	0.3
Sodium benzoate 532-32-1	5	**Benzene**	64.0	2
		Biphenyl	10.4	0.3
		Benzoic acid	5.7	0.1
		Benzophenone	3.8	0.1
		Phenol	1.7	0.04
		Toluene	0.2	*0.005*
		Styrene	0.2	*0.005*
		Benzofuran	0.2	*0.005*
Sodium citrate 68-04-2	5	Methylisobenzofuranone	13.9	0.3
		2-Butanone	5.4	0.1
		Methylcyclopentenone	5.2	0.1
		Methylbenzofuraone	4.6	0.1
		Methylfuranone	4.3	0.1
		Cresol	1.9	0.05
		Toluene	1.8	0.05
		Styrene	1.1	*0.03*
Spearmint oil 8008-79-5	21	Carvone	67.8	7
		Limonene	8.3	0.9
		β-Bourbonene	2.5	0.3
		Cineole	2.0	0.2
		Caryophyllene + ?	1.8	0.2
Starch 9005-25-8	19000	Hydroxymethylpyranone and/or hydroxymethylfurfural	52.6	5,000
		Unidentified product	12.2	1,200
		Levoglucosan	9.4	890
		Furfural	3.2	300
		Linoleic acid	2.9	280
Styrax extract (resinoid) 8046-19-3	30	Methyl styrene	47.9	7
		Cinnamyl cinnamate	36.5	5
		Benzyl cinnamate	2.8	0.4
		Cinnamic acid + β-caryophyllene	1.9	0.3
		Cinnamyl alcohol	1.7	0.3
		Styrene	0.6	0.09

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
Styrax oil 8024-01-9	5	Phenylpropene and/or methylstyrene	44.1	1
		Cinnamyl cinnamate	36.8	0.9
		Benzyl cinnamate	2.6	0.07
		Phenyl propanol	2.3	0.06
		Cinnamic acid + β-caryophyllene	2.1	0.05
		Styrene	0.7	*0.02*
Sugar, brown	56000	Hydroxymethylfurfural	49.8	14,000
		Furfural	22.1	6,200
		Formylfurfurylmethanoate	3.3	920
		Formic acid	2.0	560
		Acetyl furan	1.3	360
Sugar, invert 8013-17-0	62000	Hydroxymethylfurfural	40.1	12,000
		Furfural	34.9	11,000
		Glycoaldehyde and/or methyl formate	4.0	1,200
		Acetic acid	3.0	930
		Pyruvaldehyde	2.3	710
Sugar, white 57-50-1	25000	Hydroxymethylfurfurole	40.0	5,000
		Furfural	32.3	4,000
		Methylbenzenediol	2.4	300
		Methyl furfural	1.9	240
		Glycoaldehyde	1.8	230
		Phenol	0.3	38
		Benzene	0.2	25
		Butanal?	0.1	13
		2-Butanone?	0.1	13
		Cresol	0.1	13
		Styrene + ?	0.1	13
		Toluene	0.1	13
Tangerine extract 8016-85-1	0.5	Acetic anhydride	57.5	0.1
		Acetic acid	23.2	0.06
		Limonene	19.3	0.05
Tangerine oil 8008-31-9	1	Limonene	82.6	0.4
		γ-Terpinene	7.1	0.04
		Cymene	2.8	*0.01*
		β-Myrcene	1.3	*0.007*
		α-Pinene	0.8	*0.004*
Tea extract, absolute 68916-73-4	10	No products detected	-	-
Tea extract, distillate 84650-60-2	2.5	No products detected	-	-
Thyme oil, white 8007-46-3	5	Cymene	59.4	1
		Thymol	25.6	0.6
		Camphene	5.9	0.1
		β-Fenchyl alcohol	2.2	0.06
		Linalool and/or α-terpinolene	1.9	0.05
Tocopherols (mixed) 52-09-9	7.5	Trimethylcycloundecane	53.9	2
		Acetic anhydride	14.8	0.6
		Acetic acid	8.2	0.3
		Trimethylpentadecanone	5.8	0.2
		Tetramethylbenzoquinone	1.8	0.07
Valerian root extract 8057-49-6	560	Octalactone	11.3	32
		Unidentified compound	8.3	23
		Hydroxymethylfurfural	6.2	17
		Benzenediol	3.7	10
		Phenol	3.7	10
		Furfural	1.3	4
		Cresol?	0.4	1
Valerian root oil 8008-88-6	7.5	Bornyl acetate	40.9	2

(*Continued*)

Ingredient CAS Number	Max. cig. appln. level (ppm)	Composition of pyrolysate (Compound, %)		Max. smoke (μg)
		Camphene	14.5	0.5
		Isobicyclogermacrenol	3.9	0.1
		α-Pinene	3.2	0.1
		Limonene	1.5	0.06
Valerian root tincture 8057-49-6	100	Isovaleric acid	19.9	10
		Hydroxymethylfuraldehyde	19.6	10
		Acetic acid	18.1	9
		Valeranone	7.9	4
		Ethyl linoleate	4.9	2
		Phenol	1.3	0.7
Vanilla, absolute 8024-06-4	326	Vanillin + hydroxybenzaldehyde	68.2	110
		Ethyl linoleate	8.8	14
		Ethyl palmitate	2.7	4
		Ethyl oleate	1.5	2
		Linoleic acid	1.0	2
		Cresol	0.08	0.1
Vanilla oleoresin 8023-78-7 Diluted with glycerol and propylene glycol	326	Glycerol	92.8	150
		Vanillin	2.8	5
		Propylene glycol	1.4	2
		Guaiacol	0.7	1
		Unidentified compound	0.3	0.5
		Phenol	0.1	0.2
Verbana oil, European 85116-63-8	5	Limonene	16.7	0.4
		E-Citral	10.8	0.3
		α-Curcumene	9.7	0.2
		β-Caryophyllene	8.3	0.2
		Z-Citral	7.3	0.2
Vetiver oil 8016-96-4	0.5	Tetradehydroarisolane	10.1	*0.03*
		α-Gurjunene	7.7	*0.02*
		Tetrahydrotetramethylmethanoazuleneone	7.4	*0.02*
		Dehydroisolongifolene + cadinene + isoledene	6.6	*0.02*
		Valencene	5.8	*0.02*
Violet leaves, absolute 8024-08-6	5	Ethyl linoleolate	66.8	2
		Ethyl linoleate	13.1	0.3
		Ethyl palmitate	11.9	0.3
		Ethyl hexadecanoate	2.1	0.05
		Linalool and/or ocimene	0.8	*0.02*
Wine 91082-91-6	10	Ethyl acetate	38.5	2
		Acetic acid	30.0	2
		Acetic anhydride	13.3	0.7
		Ethanol	7.5	0.4
		Isopentanol	6.9	0.3
Xanthan gum 11138-66-2	3800	Acetic acid	34.3	650
		Acetol	13.9	260
		Caprolactone and/or hydroxyoxohexanoic acid lactone	4.3	82
		Benzenediol	3.7	70
		Corylon	2.9	55
		Furfural + cyclopentenone	2.4	46
		Phenol + methylfuranone	0.8	15
		Cresol	0.5	10
		Toluene	0.4	8
Ylang ylang oil 8006-81-3	5	Benzyl acetate	15.6	0.4
		Methyl anisole	12.5	0.3
		Germacrene	11.8	0.3
		α-Farnesene	7.6	0.2
		Caryophyllene + amorphene?	6.2	0.2

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