

APPENDIX I

In this appendix, the components measured in 33 tobacco products have been shown with their CAS number and the retention time at which the peak appeared on the chromatogram. For each product, the box is marked green when the component is present. The number in the green box represents the signal-to-noise ratio. The final columns respectively represent the components' flavour description and, if known, its odour threshold. The components numbered from 1 up to 144 (coloured blue) represent flavour additives; the components numbered from 145 up to 149 (coloured red) represent the five excluded non-flavour components; and the final components numbered from 150 up to 186 (coloured orange) are the components present in at least one of the reference products (natural tobacco leaves and/or research cigarettes containing no additives) and are therefore not considered flavour additives.

20	eugenol phenol, 2-methoxy-4-(2-propenyl)-, acetate	9 6 3 1 09 2 7- , 53- 1 0 2	1 1 1 5 3 4 7 2 8 5 7 4			Strong, spicy, dry, pungent, smoky, clove-like	6
21	α-terpineol	09 4 3- , 28- 2 7 1 09 9 8- , 55- 7 5 3	7 5 5 2 8 3 2 7 4		7 7 1 1 7 8	Sweet, spicy, balsamic-clove, fruity; warm clove-like taste	
22	β-copaene	EP 1 A- 2 36 , 03 4 30 2 16 1 72 4	3 2 3 5 4 5 6 6 6			Woody, earthy	
24	δ-cadinene <delta->	9- , 01- 2 4 9 1 1 12 3	2 2 2 7 2 9 0 5 8			Natural substances and extractives	
25	ethyl vanillin	1- , 32- 3 4 8 1 1 10 1	1 1 1 5 5 3	2 6 9 9	1 1 1 9	Intense, sweet, vanilla like odor; creamy vanilla taste	1 0 0
26	γ-triacetin	2- , 76- 7 1 8 1 1 70 3	1 1 1 2 7 3 6 6 7			Very weak ethereal-fruity odor; a mild sweet taste; normal use as solvent	
27	δ-decalactone <gamma->	6- , 14- 5 9 1 65 8 9- , 70- 3		8 8 6 2	2 8 6 8	Coconut-peach like odor; in dilution, peach taste	1 0 0
28	α-solustero	1 2 59 7 89- , 27- 2 5 6	8 8 8 8		1 1 5 9 0 1	Fruity odor of green-apple, pineapple, tropical, mango, apricot. cognac	2 0
29	β-limonene	1 1 50 0 1- , 92- 5 8 0	9 9 8 4 3 3			Tarry-medicinal phenolic spicy smoky odor	
31	γ-chavicol formic acid, phenylmethyl ester	10 7 4- , 57- 9 4 8 20 1		1 2 0 0	8 6 0 1	Strong, fresh fruity; cherry, raspberry, blueberry nuance flavor	
32	α-cadin-1(6),4-diene <trans->	08 3 5- , 11- 6 4 9 1 1 77 1	8 7 8 8 7 2			Natural substances and extractives	
33	β-guaiacol <4-vinyl-> 1h-pyrrole-2-carboxaldehyde, 1-methyl-	86- , 61- 4 0 7 11 6 92- , 58- 8 1 9 49 9	7 6 0 1		7 7	Sweet, spicy, clove-like, somewhat smoky odor; sweet taste	3
34	α-isomenthone	1 1 17 2 54- , 62- 4 7 3				Somewhat burnt, roasted, cracker, nut	3 7
35	β-isomenthone	1 1 17 2 54- , 62- 4 7 3				Strong herbaceous-minty odor; herbaceous, minty, bitter taste	9 2
36	γ-phenyl-, methyl ester, (e)-bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1r*,4z,9s*]-	1 1 11 2 8- , 65- 8 0 7		1 0 2 2	4 4 4 0	Strawberry, fruity	
37	α-1r*,4z,9s*-methylene-, [1r*,4z,9s*]-	1 1 11 2 8- , 65- 8 0 7	2 2 0 9 5 2			Woody, spicy, dry odor	
38	vanillin	12 1 1- 2	1 1 9 0	1 1 9 0		Powerful, creamy, vanilla-like odor & sweet	5 8

		6							
5		47	7						
8	eucalyptol	82-6	3-2	279					Strong, camphoraceous, cool, fresh odor
5		13	9						
9	4-(1-methyl-2-methylphenyl)-(1r,2r,5s)-5-methyl-2-(prop-1-en-2-yl)cyclohexanol	87-4	0-2				276		Sweet, herbaceous, sour, woody-lilac notes
6		29	9						
0		14	9						
		10-4	0-6	265					Natural substances and extractives
6		61	9						
1	5-(1-methylphenyl)-(-)-8-menthen-2-yl acetate, trans	01-2	7-1				265		Sweet, woody-cuminic, floral odor; minty, sweet weedy spicy taste
6		57	1						
2		28	1						
		13-5	6-3				242		unknown = (R)-dihydrocarvyl acetate
6		10	4						
3	undecalactone <gamma->	67-6	8-2				236		Strong fatty, peach-apricot odor; peach taste in dilution
6		53	4						
4	1,2-propanediol diformate	81-8	4-2				220		unknown
6		15	1						
5	5-methyl-2-(1-methylhydridene)-	93-2	0-4	218					Has an minty type odor
6		06	9						
6	benzoic acid	85-0	2-7	212					Very weak, balsamic odor and burning taste
6		14	6						
7	hexyl acetate	92-7	9-0				189		Sweet, fruity, pear-apple like odor; green, banana, apple-pear like taste
6									
8	1,2,3,4-tetrahydro-1,6-dimethyl-4-(1-methylphenyl)-, (1s-cis)-	48-3	4-3				184		Has an herbal type odor.
6		17	1						
9	menthyl lactate	16-2	3-7	173					Cooling, menthol, fresh, minty
7		29	7						
0	propanoic acid, 2-methyl-, 3-hydroxy-2,4-trimethylpentyl ester	7-0	2-3						
7		07	2						
1	terpineol <beta-, trans->	68-9	3-0				168		unknown
7		70	3						
2	decalactone <delta->	86-2	8-9				156		Sweet, creamy, milky, peach, nut; peach, buttery in dilution
7		09	4						
3	benzopyran-2-one, 6-methyl-6-octen-1-ol, 3,7-dimethyl-, propanoate	48-8	8-0				153		Coumarinic-coconut, tonka-like odor; sweet vanilla-tonka taste
7		14	3						
4		14	0						
7	isovalera	35	1	1					Sweet fruity rose odor; bittersweet, floral-green-citrus-plum-like taste Fruity, green apple odor

5	te <cis-3-hexenyl->	15 0 4 . 45- 2 1 6 10 3	4 5			and taste	
7	butyric acid	7- , 92- 8 6 2		1 4 0		Strong, cheese, butter-like, sour-rancid odor and taste	2 4 0 1
7	isophorone	07 8 8- , 59- 6 1 8		1 3 8		Sharp, sweet-green-camphoraceous odor; minty-honey-tobacco on dilution	1 0 0 0
7	2h-pyran-2-one,	69 1					
8	tetrahydro-6-propyl-2(3h)-furanone, 5-butylidihydro-4-methylacetic acid, phenyl-, isopentyl ester	8- , 76- 0 0 8 39 1 21 1 2- , 23- 6 2 1 10 3 2- , 19- 7 2 9				Coumarinic, coconut odor, creamy, coconut flesh taste	4 0 0
7	3-hexen-1-ol, formate, (z)-	33 46 4 7- , 73- 6 1 9 30 1				Coumarinic, coconut, lactonic, woody, maple and lovage	4 6
8	muurole ne <gamma->	02 3 1- , 74- 7 0 3		1 3 0		Sweet, balsamic-floral-fruity-apple; honey notes; reminiscent of cocoa bean	
8	octalactone <gamma->	10 0 4 . 50- 6 7 7		1 3 0		Strong, sharp, green fruity-apple; green fruity vegetable taste	
8	2(3h)-furanone, dihydro-5-propyl-	10 9 5- , 21- 1 5 3 1				Has an woody type odor = gamma muurole ne	
8	ionone <(e)-, beta->	07 3 9- , 77- 7 6 9 40 1				Sweet-coumarinic, coconut-like odor and taste	4 0 0
8	nerolidol <(e)->	71 4 6- , 66- 6 3 6 54 7				Coconut, hay-like, coumarinic odor	4 0 0
8	methyl isobutyrate	7- , 63- 5 7 9		1 1 4		Woody, violet, fruity odor; woody-raspberry on dilution	0 6
8	2-cyclohexen-1-one, 3-methyl-6-(1-methylethyl)-2(3h)-furanone, dihydro-5-methyl-1,3-dioxolane-2-acetic acid, 2,4-dimethyl-, ethyl ester	10 6 8- , 29- 1 2 1 1 62 0 90- , 17- 2 1 7 1				Faint, woody-floral, slight green odor; weak green floral taste	1 2 0
8	nonanoic acid, ethyl ester	12 1 3- , 29- 0 5 8 54		1 1 4		Fruity, apple-pineapple-apricot-rum like odor and juicy fruit taste	7
8	ethanol, 1-(2-butoxyethoxy)-benzaldehyde propylene glycol acetal	44 9 6- , 78- 5 5 9 1 25 0 68- , 25- 8 4 4				Fresh strong herbaceous, minty	6 8 0
9						Sweet, hay-like, coumarinic odor and coconut taste	1 0 0 0
9						Fresh, sweet-fruity notes reminiscent of apple and strawberry	
9						Fatty-waxy, oily, cognac, grape, nut-like odor; wine-cognac tropical taste	8 5 0
9						Natural substances and extractives	
9						Practically odorless; faint cherry, bitter almond	

176	2,3-pentanedione	0 2 60 3 14-0 6 6	1 1 1 1 1 3 2 1 1 2 9 8 8 6 2 5 2 5 2 3 5	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 3 3 3 4 1 1 1 0 0 1 1 6 2 6 9 9 9 2 0 3 5 2 9 1 6	1 1 9 0 1 9 1 4	1 1 1 2 9 7	Oily-buttery, fatty odor; butter, cream, milk taste	2 0	
177	4h-pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	28 56 8 4- 83-9 2 9	1 1 1 1 1 7 2 6	1 0 9 6 4	1 1 8 8 6 8 7 8 1 3	1 1 1 0 7 7	unknown		
178	ethanone, 1-(2-furanyl)-	92- 62-4 7 7	1 1 1 3 3 1 7 3 7	1 1 1 1 1 1 2 1 8	1 1 1 1 1 1 1 1 4 4 4 5 2 2 3 9 6 8 7 4 2 8 3	1 0 9	Has a balsamic type odor and an nutty type flavor	2 0 0	
179	butyrolactone	09 5 6- 48-5 0 3	9 8 2 8	8 3	7 7 7 9	8 4	8 8 8 2 3 2	Weak, slightly caramellic, nutty, buttery odor	0 0
180	furan-3-one <2-methyl-, tetrahydro->	31 4 88- 00-1 9 1	9 8 7 7 7 6 0 0 8 5 4 7	6 0	7 9 9 9 9 7 7 8 6 6 3 2 4 9 8 4 2 3 5 1 0	7 7 8 5 6 7 9 8 8 7 6 7 9 4 1	Sweet and solvent-like odour, nutty and astringent flavour with a creamy almond nuance		
181	5,9-undecadien-2-one, 6,10-dimethyl-, (e)-naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	1 37 3 96- 70-2 1 5	1 9 0 9 7 8 6 8 0 7 8 7 0 8 1 7 1 3 1	1 9 8 3 5	1 1 1 1 1 1 1 0 0 0 0 0 0 0 7 8 7 8 1 0 5 3 6	7 7 9 8 4 6 6 6 0	A fresh, rose, magnolia-type odor		
182	1,4-benzene diol, 2-methyl-2-buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (e)-	1 47 0 5- 03-6 6 9	8 7 7 6 7 7 1 6	6 7	6 6 6 7 7 7 8 5 9 9 8 0 5 2 0 8	6 6 1 5	6 6 8 5 7 0 7 2 8 3	unknown	
183	1,4-benzene diol, 2-methyl-2-buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (e)-	09 7 5- 71-9 6 2					6 6	unknown	
184	pyrrole <2-acetyl->	23 1 72 2 6- 93-4 4 6	6 5	6 5	7 5 7 6 5 5 9 6 1 7	5 7	6 1	Has a floral type odor and an woody type flavor	
185	propanone, 1-(acetyloxy)-	10 7 72- 83-6 9 7	8 9 6 8 8 6 2 1 8 3 8 4	8 4	8 8 8 8 8 8 9 6 6 6 4 6 6 6 0 9 5 3	7 0	6 7 7 9 5 3 0 5 1 7	Has a musty type odor and an nutty type flavor	
186	propanone, 1-(acetyloxy)-	59 4 2- 20-8 1 3	5 6 3		6 6 6 5 5 6 4 6 4 8 9 2	5 9	6 6 0 8	unknown	

