

VOLATILE CONSTITUENTS OF PERIQUE TOBACCO

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KEY WORDS

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ABSTRACT

The volatile constituents of Perique tobacco were determined by GC-MS. In excess of 330 components were identified. The distinct aroma of Perique is due to the extensive formation of components derived from the unique curing process of high-pressure anaerobic fermentation. 48 new tobacco constituents were identified.

Plant Name:

Nicotiana tabacum

Source:

Commercial sample of Perique tobacco produced in St. James Parish, Louisiana, USA.

Plant Part:

Granulated leaves after curing by high-pressure anaerobic fermentation.

PREVIOUS WORK:

No analysis of the volatile constituents of Perique tobacco has previously been published.

INTRODUCTION:

Perique tobacco is a minor tobacco type produced by subjecting the leaf of a Red Burley (USDA Type 72) to a partial air-curing followed by a high pressure anaerobic fermentation process.

Genuine Perique grows successfully only in a small, wedge shaped piece of land west of New Orleans called St. James' Parish. Within St. James' Parish, the best, and only current location the Red Burley for Perique is grown is a relatively tiny place called Grande Point Ridge, near Paulina, LA. on a dark alluvial soil.

Growers have tried sowing the Red Burley seed in places all over the world with similar climate and soil conditions without any significant success other than Kentucky Green River Burley, which can be grown in larger crops, and is processed to make a “faux” (**fake**) Perique.

In 2002, the world's production of pure Perique -11,460 pounds - was stored in 27 oak whiskey barrels at the last producers farm [1,2]. It is estimated that an additional amount of about 50,000 pounds of the Acadian Green River “faux” Perique is produced. Although several hundred thousand pounds of “genuine” Perique was produced at one time, it is likely that its production will cease at some point in the near future due to its labor intensity, changing demographics, and economics.

The process used to produce Perique is essentially the same as introduced commercially in the 1820's by Pierre Chenet who had observed the Choctaw Indians smoking a tobacco that had been fermented under pressure in tree stumps using a press and a lever. The tobacco is harvested in late June and cured with air-drying, though for a shorter time than standard Burley. After air drying for about three weeks the main veins (or midribs) are removed by hand; the leaves then being tied into 'torquettes' or tight bundles of approximately 1 pound (450 g). These are pressed in large oak whiskey barrels with very heavy pressure, the 'juices' being collected as they seep out of the top of the press. The torquettes are turned and returned to the press (along with the “juices”) a number of times over the better part of a year, fermenting “anaerobically”, or without air. The whole process takes about a year at the very minimum and is highly labor intensive in relation to curing other strains of tobacco [3]. This, in combination with the limited crop supply, makes Perique rare, and very expensive.

Although the major tobacco types (Virginia, Burley, Oriental) have been the subjects of extensive chemical investigation, no analysis of Perique has previously been published.

EXPERIMENTAL:

Sample Preparation: A “TEABAG” (1 ½ “ X 1 ½ “) was constructed from unscented tissue paper. 100 grams of prebaked-out Tenax TA (20-35 mesh) was placed in the Teabag and the Teabag was suspended above 10 grams of Perique Tobacco (in a 16oz jar) for 28 hours.

The Tenax was then removed and packed into an injection port liner (glass-wool plugs on top and bottom). The Liner was then placed in the GC injection port for direct injection of the volatiles into the GC.

GC and GC/MS: The GC-MS was a Hewlett-Packard 6890/5973 High Performance combination. A HP-5ms 60m X 0.32mm I. D. fused silica column coated with a .25 micron film thickness (HP part No. 19091S-416) was used in this analysis. The column was held isothermally at 30°C for 2 minutes, then programmed from 30°C to 260°C at 2C/min, with a final hold time of 28 minutes to give a total analysis time of 145 minutes. The Injection port was held at 260°C. Helium Carrier Gas was used with a flow rate of 3.5 ml/min. The Mass spectrometer was scanned in the EI mode from 26m/z to 350m/z using 70eV ionizing voltage.

Component Identification: Identifications were based on mass spectra from the Wiley 6 and NIST 98 MS libraries as well as from the authors MS library. Where available, retention time comparisons were used (as well as employing the RI index of Boelens [4] and other published sources.

Initial analysis was done on the HP MS Enhanced Chemstation program employing both normal and selective ion modes. The NIST Amdis deconvolution program (Version 2.6) was also employed in both normal and high resolution modes using the MSP file format from data imported from the Wiley 6 and NIST 98 MS libraries, as well as the authors library. Percentages are based on FID response. For overlapping peaks, percentages were apportioned based on the AMDIS peak purity percentages.

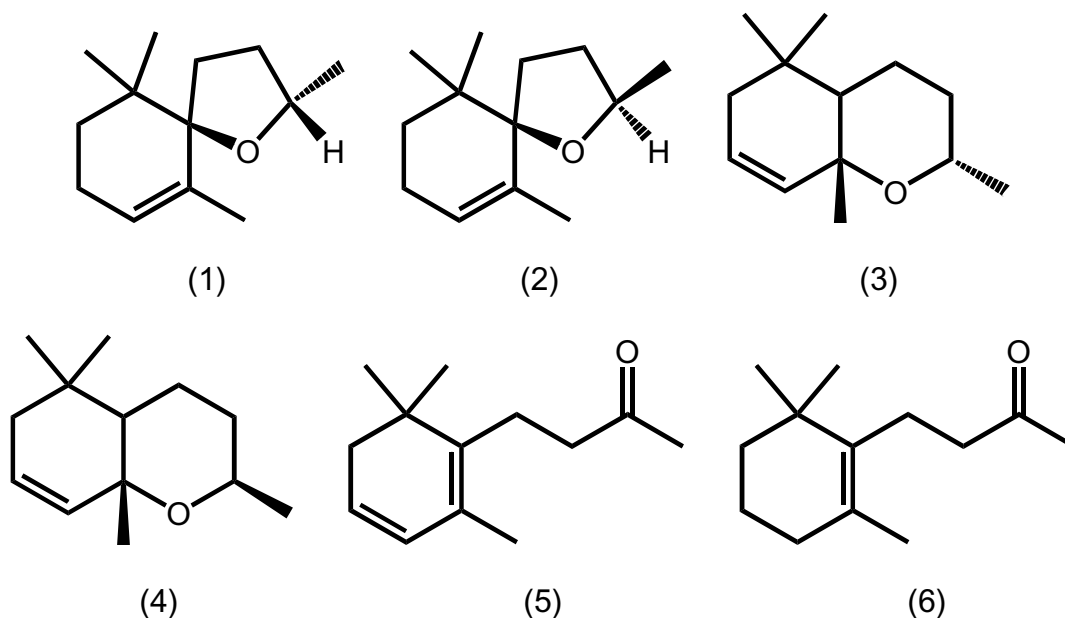
RESULTS & DISCUSSION:

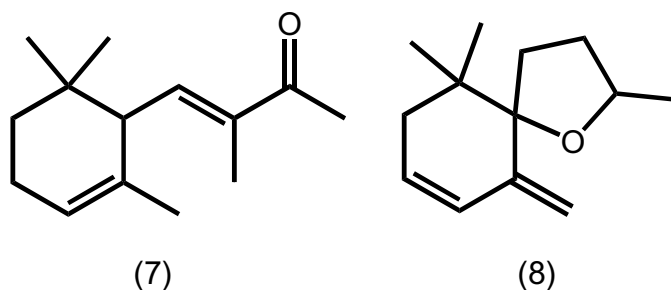
Although the chemical composition of the major tobacco types (Virginia, burley and Oriental) have been extensively studied [5-13], only recently have the minor tobacco types of fire-cured and Latakia received any attention [14,15].

Perique is the last tobacco type that has never previously been analyzed. In this study, 334 constituents were identified comprising 97.48% of the volatiles (see Table 1). 48 new tobacco leaf isolates were identified [16].

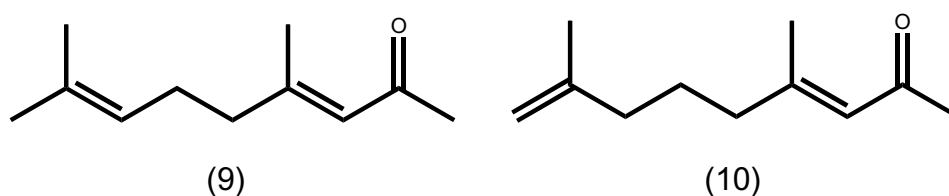
New Tobacco Isolates:

26 of the new tobacco isolates were alcohols and esters commonly found in fermented products, e.g., esters of acetic, propionic, isobutyric, 2-methylbutyric and isovaleric acids with isoamyl alcohol & 2-methylbutan-1-ol, and several new alcohol isolates.

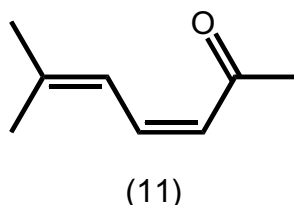




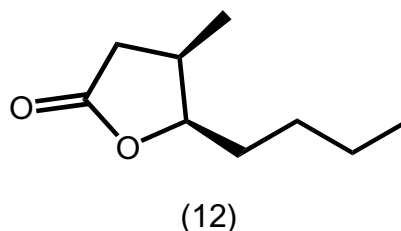
Several carotenoid degradation products not previously found in tobacco were present, notably – Theaspirane “A” (1), Theaspirane “B” (2), Dihydroedulan I (3), Dihydroedulan II (4), 4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)butan-2-one (5), and Dihydro-beta-ionone (6). alpha-iso-Methylionone (7) and Vitaspirane (8) were tentatively identified.



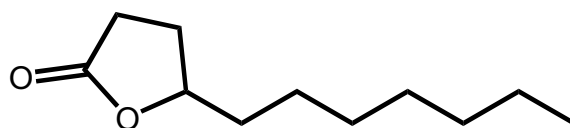
4,8-Dimethylnona-3,7-dien-2-one (9), which can be considered an aldol condensation product of 6-Methyl-5-hepten-2-one and acetone, and the 3,8-diene isomer (10) were also present.



Although (E)-6-Methyl-3,5-heptadienone is a common tobacco constituent, in this study we also found an equal amount of the previously unreported (Z)-isomer (11).

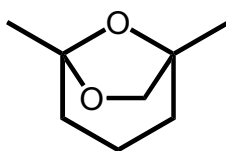


cis-Oak lactone (12), also known as whiskey lactone, was isolated; this presumably was generated by the whiskey barrel used in the high pressure fermentation.



(13)

Gamma-Undecalactone (5-Butyl-4-methyldihydrofuran-2(3H)-one) (13), which possesses a fruity-peach like note, was also identified in tobacco for the first time.



(14)

Surprisingly, Frontalin (14), the aggregation pheromone of the Southern Pine Beetle, was also present.

Two new sesquiterpenes were also isolated (alpha- & gamma-Muurolene), along with benzopenone, 1,2-Diphenoxyethane, 2,6-Di-tert-butylbenzoquinone and 2-Ethoxybutanol. Eucarvone (2,6,6-Trimethyl-2,4-Cycloheptadien-1-one) is also a new tobacco isolate.

The odor descriptors in the Table 1 of constituents are those of Leffingwell [17] or Boelens [18].

CONCLUSIONS:

Static headspace analysis of Perique tobacco by GC-MS provides a rapid and convenient method for the identification of the complex tobacco volatiles. The use of the NIST Amdis program allows the automated and accurate identification of overlapping constituents in mixed GC peaks. The characteristic aroma of Perique is due in part to the generation of large amounts of classical fermentation alcohols and esters. More than 14% of the 334 components identified are new tobacco isolates.

Acknowledgements: We thank Ms. Marlene Adams of Brown and Williamson Tobacco Corporation for providing us with the sample of Perique tobacco.

Table 1: Volatile Constituents of Perique Tobacco

RI _(calc) - HP5	Actual R.T.	Constituent	%	ID	Odor Description
367.5	2.843	Methanol	0.072	MS	
401.1	2.970	Methyl formate	0.014	MS	Fresh, warm ethereal, winey- rum-chloroform-like
427.0	3.072	Ethanol	0.074	MS, RI	Sweet, ethereal (alcoholic) odor
476.6	3.277	2-Propanone	0.355	MS	Characteristic solvent odor
483.4	3.306	2-Propanol	0.032	MS	Characteristic "rubbing-alcohol" odor
505.0	3.499	Dimethyl sulfide	0.008	MS, RI	Pungent, cabbage, cooked vegetable odor
515.3	3.587	Methyl acetate	0.932	MS	Sweet, volatile ethereal-fruity odor
556.0	3.893	2-Methylpropanal	0.055	MS, RI	In dilution, pleasant, fruity, chocolate, banana-like odor
557.9	3.915	1-Propanol	0.029	MS	Alcoholic, sweet odor; bland fruity notes
559.6	3.934	2-Methylpentane	0.015	MS	
580.8	4.191	3-Methylpentane	0.011	MS	
592.4	4.331	2,3-Butanedione	0.015	MS, RI	Strong, buttery odor
601.8	4.451	2-Butanone	0.313	MS, RI	Sweet, solvent, acetone-like ketonic odor
609.0	4.547	2-Butanol	0.038	MS	Oily, wine-like, fusel-alcoholic note
611.1	4.574	3-Methylfuran	0.063	MS	
615.2	4.630	2,3-Dimethyl-1-butene	0.010	MS	
623.7	4.746	2-Methyl-3-buten-2-ol	0.105	MS	Sweet, oily-fruity, herbaceous- earthy
626.1	4.780	2-Methylfuran	0.061	MS	Sweet-gassy, solvent, metallic- burnt with musty notes
628.0	4.821	Ethyl acetate	0.189	MS, RI	Ethereal, sharp, wine-brandy like odor
637.2	5.068	2-Methylpropanenitrile	0.007	MS	
642.5	5.217	2-Methyl-1-propanol	2.181	MS, RI	Breathtaking, sweet, sweaty- chemical; whiskey-like
642.6	5.220	Methyl propionate	0.242	MS	Ethereal, fruity, rum-like odor
661.0	5.770	3-Methylbutanal	0.227	MS, RI	Powerful, penetrating; cheesy- sweaty-fruity in dilution
666.1	5.933	3-Methyl-2-butanone	0.051	MS	
669.7	6.049	2-Methylbutanal	0.190	MS, RI	Strong, breathtaking odor; cocoa- like, weak fruity on dilution
673.0	6.159	Acetic acid	0.082	MS, RI	Pungent, sour, vinegar odor
688.8	6.713	1-Penten-3-ol	0.087	MS, RI	Pungent, grassy, alliaceous-like; green vegetable, fruity
691.6	6.814	Methyl isobutyrate	0.127	MS, RI	Fruity, apple-pineapple-apricot-rum like odor

701.3	7.185	3-Pentanone	0.176	MS	Ethereal, mild acetone-like; slight fruity cheese note
704.8	7.322	2-Ethylfuran	0.047	MS, RI	Strong, sweet-ethereal, burnt brown musty odor
713.8	7.688	Acetoin	0.031	MS, RI	Creamy-buttery, yogurt-like odor
717.2	7.835	Ethyl propionate	0.020	MS, RI	Strong, ethereal, fruity, rum-like odor
720.1	7.957	Propyl acetate	0.015	MS	Sweet, ketonic, fermented, fruity, caramellic notes
723.0	8.307	Methyl butanoate ^a	0.012	MS, RI	Sweet, ethereal fruity odor; apple-like
730.4	8.637	3-Methylbutanenitrile	0.009	MS	
731.6	8.692	Pyrazine	0.042	MS	Pungent, sweet, corn-like, roasted hazelnuts
752.5	9.700	Pyridine	0.042	MS, RI	Strong, amine-like, fishy, burnt odor
759.3	10.055	Isoamyl alcohol	32.802	MS, RI	Breathtaking, alcoholic odor; in dilution winey-brandy
763.0	10.252	2-Methylbutan-1-ol	0.893	MS, RI	Ethereal, fusel oil, fermented winey notes
766.1	10.421	Toluene	0.096	MS, RI	
779.5	11.180	Isobutyl acetate ^a	0.171	MS, RI	Strong, fruity, banana-pear notes
780.0	11.209	1-Pentanol	0.171	MS, RI	Alcoholic-breathtaking, fusel-like odor
781.3	11.289	Methyl isovalerate	0.091	MS, RI	Strong, fruity, ethereal, apple-like odor
781.7	11.310	Methyl 2-methylbutyrate ^a	0.100	MS, RI	Fruity, sweet, apple, berry, ripe and pineapple
782.7	11.368	cis-2-penten-1-ol	0.114	MS, RI	Fresh, ethereal, fruity-green, citrus, somewhat metallic
786.6	11.605	3-Methyl-2-buten-1-ol (Prenol)	0.038	MS, RI	Fruity, green
792.9	11.995	Isoamyl formate ^a	0.052	MS	Sweet, green-fruity-winey resembles blackcurrant, plum & apple
801.1	12.524	Mesityl oxide	0.105	MS	Minty with honey-bread like notes
803.9	12.712	Isobutyric acid	0.015	MS	Sour cheesy odor; In dilution a fruity odor
807.1	12.929	4-Methyl-2-pentanol	0.023	MS	Oily-green-winey, fusel-fermented alcoholic notes
812.6	13.306	2-Hexanol ^a	0.033	MS	Weak, fruity, fatty, fermented notes
817.0	13.617	Butyl acetate	0.012	MS, RI	Strong, sweet, fruity; banana, pear, pineapple notes
820.0	13.832	2-Methylpyridine	0.032	MS	Astringent, hazelnut-popcorn and rum-like
827.0	14.055	2-Methylpyrazine	0.207	MS, RI	Green, nutty, cocoa, musty, potato, fishy-ammoniacal notes
829.1	14.190	Methyl valerate	0.023	MS, RI	Ethereal, green-fruity, apple-pineapple like odor
835.2	14.586	2,3-Dimethyl-1-butanol ^a	0.015	MS	

838.2	14.780	Furfural	0.009	MS, RI	Sweet, cereal, bread-like, yeasty, caramellic, spicy notes
843.0	15.103	2-Methyl-1-pentanol ^a	0.029	MS	Sweer ethereal, alcoholic with fusel-fermented notes
846.2	15.323	4-Methyl-1-pentanol	0.034	MS	Oily green-fruity, herbaceous, yeasty-fermented note
849.4	15.543	4-Hydroxy-4-methyl-2-butanone ^a	0.038	MS	
854.5	15.904	3-Methyl-1-pentanol	0.009	MS	Winey, cognac, whisky, fruity, green notes
856.4	16.040	Ethyl 2-methylbutyrate	0.010	MS, RI	Strong, green, fruity, apple-strawberry odor
856.6	16.060	2,4,5-Trimethyloxazole	0.018	MS	Boiled beef, nutty, sweet, green
859.3	16.256	Ethyl isovalerate	0.027	MS, RI	Strong, fruity apple odor
863.3	16.550	Ethylbenzene	0.015	MS, RI	
863.9	16.594	cis-3-Hexenol	0.043	MS, RI	Strong, fresh, green, grassy odor
865.9	16.741	Furfuryl alcohol	0.031	MS, RI	Weak, fermented, burnt-sugar, creamy, caramellic notes
866.4	16.782	3-Methylpyridine	0.016	MS	Green earthy with hazelnut notes on dilution
867.8	16.887	4-Methylpyridine	0.039	MS	
868.2	16.914	4-Methyl-3-penten-1-ol ^a	0.129	MS	
871.2	17.149	m-Xylene	0.073	MS, RI	
873.6	17.329	Butyl propanoate ^a	0.046	MS	Ethereal, fruity, rum odor
878.1	17.683	1-Hexanol	0.257	MS, RI	Chemical, winey, slight fatty-fruity odor
882.6	18.052	Isoamyl acetate ^a	0.659	MS, RI	Sweet, fruity, banana, pear odor
884.5	18.204	2-Methylbutyl acetate ^a	0.241	MS, RI	Ethereal rum-like fermented-fruity odor; banana
887.2	18.424	2,6-Dimethylpyridine	0.132	MS	Green, nutty, herbaceous-pyridine, musty, coffee-cocoa
888.7	18.548	Isovaleric acid	0.070	MS, RI	Very sour, "sweaty", cheesy, odor
891.4	18.776	Styrene ^a	0.045	MS, RI	Characteristic resinous-balsamic pungent hydrocarbon odor
893.7	18.971	2-Heptanone	0.118	MS, RI	Fruity, cheese, cinnamon odor
898.3	19.366	2-Methylbutyric acid	0.251	MS, RI	Pungent, acrid, Roquefort cheese like; fruity in dilution
905.1	19.967	2-Heptanol ^a	0.015	MS, RI	Green, lemon, herbaceous odor
905.7	20.025	2-Ethylpyridine	0.039	MS	Fishy, green, grassy, smoke notes
908.6	20.285	2-Ethoxybutanol ^a	0.040	MS	
910.4	20.450	2,5-Dimethylpyrazine	0.178	MS, RI	Chocolate, roasted nuts, earthy
911.2	20.530	2-Acetylfuran	trace	MS, RI	Sweet, balsamic, cereal, slight nut notes
911.4	20.545	2,6-Dimethylpyrazine	trace	MS, RI	Chocolate, roasted nuts, fried potato odor
913.8	20.772	Dihydrofuran-2(3H)-one+ 2-ethylpyrazine	0.161	MS	
917.1	21.076	2,3-Dimethylpyrazine	0.150	MS, RI	Green, nutty, potato, cocoa, coffee, caramel, meaty notes

923.2	21.669	Methyl hexanoate	0.035	MS, RI	Ethereal fruity (pineapple-apple) odor
940.0	22.038	alpha-Pinene	0.017	MS, RI	Resinous, pine odor
941.3	22.157	2,4-Dimethylpyridine	0.015	MS	Pyridine animalic, fishy-minty-like; green in dilution
943.3	22.336	2-Methyl-5-isopropenylfuran ^{a,b}	0.030	MS	
949.2	22.869	Frontalin (1,5-Dimethyl-6,8-dioxabicyclo[3.2.1]octane) ^a	0.041	MS	
952.2	23.154	2,3-Dimethylpyridine	0.038	MS	roasted, rubbery
953.1	23.234	2-Methylcyclohexanone	0.024	MS	Ketonic, cooling, minty-almond
957.4	23.640	3-Methyldihydrofuran-2(3H)-one	0.273	MS	
957.9	23.690	n-Propylbenzene	0.008	MS	
962.1	24.094	5,5-Dimethylfuran-2(5H)-one	0.054	MS	
962.3	24.120	5-Methyldihydrofuran-2(3H)-one	0.323	MS	Sweet, hay-like, coumarinic odor
964.9	24.371	Benzaldehyde	0.313	MS, RI	Odor of bitter almond oil; characteristic sweet cherry
969.0	24.783	A Ethylmethylpyridine	0.042	MS	
971.2	25.000	3-Methylpentanoic acid	0.080	MS	Cheesy, sweaty odor
971.5	25.033	3-Ethenylpyridine	0.091	MS	
973.9	25.272	Isoamyl propionate ^a	0.065	MS	Sweet, fruity, apricot-banana-pineapple-plum notes
974.3	25.320	Sabinene	0.026	MS, RI	Spicy terpenic citrusy
975.6	25.449	2-Methylbutyl propionate ^a	0.026	MS	Sweet, banana, fruity, tutti-fruitti, apple, melon, tropical
979.0	25.470	beta-Pinene	0.015	MS, RI	Dry, woody, resinous-piney odor
983.5	25.827	1-Ethyl-2-methylbenzene	0.005	MS	
989.9	26.340	Benzonitrile	0.065	MS	Cherry, bitter almond like
991.7	26.482	5,5-Dimethyldihydrofuran-2(3H)-one	0.056	MS	
995.4	26.790	6-Methyl-5-hepten-2-one	0.958	MS, RI	Oily-green, herbaceous odor
996.8	26.900	beta-Myrcene	0.020	MS, RI	Resinous terpene odor
997.2	26.940	2-Pentylfuran	0.034	MS, RI	Ethereal rum; earthy beany with vegetable notes
997.5	26.960	1,2,3-Trimethylbenzene	0.025	MS	
998.9	27.079	2-Octanone	0.044	MS, RI	Fatty, green, fruity, cheese-apple odor
1002.9	27.416	6-Methyl-5-hepten-2-ol	0.415	MS, RI	Weak, sweet, oily-green; reminiscent of coriander
1003.0	27.420	2-Ethyl-6-methylpyrazine	0.232	MS	Roasted, nutty, cocoa like notes
1007.8	27.848	Trimethylpyrazine	0.201	MS, RI	Nutty, baked potato, roasted peanut, cocoa, burnt notes
1009.2	27.946	Isobutyl 2-methylbutyrate	0.023	MS, RI	Sweet fruity odor
1010.0	28.020	1-Methyl-1H-pyrrole-2-carboxaldehyde	0.003	MS	
1012.0	28.190	3-Pyridinecarbonitrile + delta-3-carene	0.062	MS, RI	
1012.7	28.248	Isobutyl isovalerate ^a	0.019	MS	Fruity, apple-raspberry like odor
1014.4	28.401	1,2-dichlorobenzene	0.017	MS	

1018.3	28.746	Isoamyl isobutyrate ^a	0.071	MS	Strong mixed fruit odor
1021.5	29.027	2-Methylbutyl isobutyrate ^a	0.035	MS	Strong mixed fruity odor
1021.8	29.050	alpha-Terpinene	0.005	MS, RI	Refreshing, lemony-citrusy terpene odor
1024.5	29.297	A Trimethylbenzene	0.028	MS	
1027.1	29.527	p-Cymene	0.056	MS, RI	Strong, characteristic, terpene odor; oxidized lemon note
1030.9	29.880	Limonene	0.734	MS, RI	Fresh, sweet, hydrocarbon and orange citrus odor
1032.5	30.024	Eucalyptol (1,8-cineole)	0.001	MS, RI	Strong, camphoraceous, cool, fresh odor
1034.8	30.240	2-acetylpyridine	0.005	MS	Popcorn odor
1035.9	30.340	2,2,6-trimethylcyclohexanone + unknown	0.108	MS	Thujone-like, camphoraceous tobacco notes
1037.5	30.494	trans-3,4-Dimethylbutyrolactone	0.020	MS	
1038.8	30.613	2-Acetyl-5-methylfuran	0.025	MS	Nutty, hay, caramel, coumarin odor
1039.3	30.656	2,3-Dihydroindole	0.078	MS	
1041.3	30.918	Benzyl alcohol + 2-hydroxybenzaldehyde	1.618	MS, RI	Pungent, irritating phenolic-almond odor
1043.0	31.010	5-Ethenyldihydro-5-methyl-2(3H)-Furanone	0.071	MS	Weak, fruity-floral with peppermint connotation
1045.5	31.249	1-Methyl-2-pyrrolidinone	0.013	MS	
1049.5	31.638	Phenol	0.260	MS	Phenolic medicinal odor
1055.2	32.193	5-Ethyldihydrofuran-2(3H)-one	0.361	MS, RI	Coumarin-like, sweet odor
1056.0	32.272	gamma-Terpinene	0.075	MS, RI	Refreshing herbaceous-citrus like terpene odor
1057.1	32.385	2,6,6-Trimethyl-2-cyclohexenone	0.268	MS	Sharp, herbaceous-camphoraceous odor; thujone-tobacco notes
1065.0	33.018	Acetophenone	0.348	MS, RI	Sweet, pungent, harsh, cherry-like odor
1070.2	33.400	(E,Z)-3,5-Octadien-2-one	0.017	MS, RI	
1072.3	33.560	cis-Linalool oxide (5) (furanoid)	0.242	MS, RI	Sweet, floral, creamy, woody, slight earthy
1075.1	33.770	An Ethyldimethylbenzene	0.010	MS	
1077.3	33.938	Benzyl formate	0.026	MS, RI	Strong, fruity-cherry, green odor
1078.6	34.035	2-Ethyl-3,5-dimethylpyrazine	0.008	MS	Cocoa, chocolate, nutty (burnt almond) notes
1086.4	34.630	an Ethyldimethylpyridine	0.167	MS	
1086.5	34.640	Terpinolene	0.055	MS, RI	Sweet, piney, slightly anisic, somewhat pleasant odor
1088.6	34.806	trans-Linalool oxide (5) (furanoid)	0.173	MS, RI	Sweet, floral, creamy, leafy earthy
1092.4	35.097	2-Nonanone	0.023	MS, RI	Fruity, fatty-cheese odor
1093.6	35.196	(E,E)-3,5-Octadien-2-one	trace	MS, RI	Woody, pleasant mushroom
1094.6	35.270	Methyl benzoate	0.136	MS, RI	Pungent, heavy, sweet, fruity-floral odor
1097.0	35.460	Heptanoic acid	trace	MS, RI	Fatty, sour-sweat-like, rancid odor
1100.0	35.594	Undecane	0.049	MS, RI	

1100.5	35.743	Isoamyl 2-methylbutyrate ^a	0.087	MS, RI	Strong fruity ripe banana-apple odor
1103.4	35.970	Linalool	0.143	MS, RI	Floral-citrusy (lime)
1104.4	36.050	2-Methylbutyl 2-methylbutyrate ^a	0.043	MS, RI	Fruity, apple, rum, berry odor
1105.7	36.160	(Z)-6-Methyl-3,5-heptadienone ^a	0.060	MS	
1106.4	36.216	Isoamyl isovalerate ^a	0.050	MS, RI	Fruity odor reminiscent of apple
1107.4	36.297	(E)-6-Methyl-3,5-heptadienone	0.060	MS	Spicy, cinnamon-nut like odor
1108.7	36.401	2-Methylbutyl isovalerate ^a	0.045	MS, RI	Herbaceous, fruity, winey-earthly apple odor
1109.1	36.436	3-Acetylpyridine	0.672	MS	Strong, somewhat choking, cigar-tobacco like odor
1117.1	37.085	2-Phenethyl alcohol	3.644	MS, RI	Floral, rose-like odor; floral taste
1118.3	37.185	A Tetramethylbenzene	trace	MS	
1120.9	37.407	Isophorone	0.577	MS, RI	Sharp, sweet-green-camphoraceous odor
1136.6	38.736	Methyl 3-pyridinecarboxylate	0.048	MS	Sweet, herbaceous tobacco-like odor
1138.1	38.870	Benzeneacetonitrile	0.060	MS	
1142.1	39.219	4-Ketoisophorone	0.168	MS, RI	Tobacco, hay-straw, tea notes
1143.9	39.378	5-Ethyl-6-methyl-3(E)-hepten-2-one	0.046	MS	
1149.8	39.900	Menthone	0.071	MS, RI	Minty-herbaceous (not green); dry woody notes
1155.5	40.403	2-Ethyl-3,5,6-trimethylpyrazine	0.052	MS	
1163.0	40.772	Benzyl acetate + unknown	0.103	MS, RI	Sweet, floral, fruity odor of jasmin and gardenia
1168.5	41.123	3,5,5-Trimethyl-1,4-cyclohexanedione	0.091	MS	Weak, sour
1168.5	41.128	1,5,5-Trimethyl-9-oxa-bicyclo[4.3.0]non-2-ene	trace	MS	
1170.8	41.272	Ethyl benzoate	0.029	MS, RI	Floral, fruity odor
1171.7	41.330	3-Methylacetophenone	trace	MS	
1173.7	41.462	Menthol	0.061	MS, RI	Trigeminal cooling sensation; slight mint note
1176.0	41.615	Phenethyl formate ^a	0.063	MS, RI	Strong, green, herbaceous, rose odor
1178.1	41.750	1-Terpinen-4-ol	0.010	MS, RI	Sweet, earthy-green, musty; slightly peppery woody notes
1178.9	41.803	Methyl phenylacetate	0.053	MS, RI	Strong, sweet floral-honey odor
1182.6	42.048	Naphthalene	0.069	MS, RI	Characteristic dry tarry hydrocarbon odor
1186.1	42.276	4-Methylacetophenone	0.035	MS, RI	Harsh, but sweet, floral-hay odor
1197.5	43.037	Methyl salicylate	0.072	MS, RI	Warm, sweet, wintergreen odor
1200.4	43.236	trans-Dihydrocarvone	0.022	MS, RI	Minty rye like odor
1200.0	43.329	Dodecane	0.014	MS, RI	Mild aliphatic hydrocarbon odor
1201.0	43.400	Safranal	0.035	MS	Powerful saffron aroma; tobacco-camphoraceous notes
1218.2	44.579	(E)-3-Methylnon-2-en-4-one	0.032	MS	
1222.7	44.896	2,6,6-Trimethyl-2,4-Cycloheptadien-1-one (Eucarvone) ^a	0.044	MS	

1223.9	44.982	beta-Cyclocitral	0.040	MS, RI	Sweet, mild green, grassy floral hay-like odor
1225.1	45.060	3-Phenylfuran	0.021	MS	
1227.3	45.218	Methyl nonanoate + unknown	0.027	MS, RI	Fruity-winey, green, nut-coconut like odor
1240.3	46.148	Quinoline	0.009	MS	Heavy, sweet, nauseating odor; animal like in dilution
1240.8	46.186	4,8-Dimethylnona-3,7-dien-2-one ^a	0.002	MS	Fruity, fresh, acetate, rose oxide, aqueous grapefruit, melon
1242.0	46.273	Vitispirane (2,10,10-trimethyl-6-methylene-1-oxaspiro[4.5]dec-7-ene) ^{a,b}	0.001	MS	
1245.3	46.510	2-Phenoxyethanol	0.035	MS	Fain floral-rose odor
1250.5	46.723	Carvone + unknown	0.043	MS, RI	Minty, spearmint/caraway
1255.9	47.284	1,2,3,4-Tetrahydro-1,1,6-trimethylnaphthalene (alpha-ionene)	0.023	MS	
1259.4	47.550	Linalyl acetate ^a	trace	MS, RI	Sweet, floral, fruity odor
1261.4	47.695	Phenethyl acetate	0.121	MS, RI	Sweet, rose, fruity, honeylike odor
1266.0	48.036	5-Butyldihydrofuran-2(3H)-one	0.085	MS, RI	Sweet-coumarinic, coconut-like odor
1272.4	48.520	PG acetal of benzaldehyde	0.078	MS	Practically odorless; faint cherry, bitter almond
1277.3	48.895	4,8-Dimethylnona-3,8-dien-2-one ^a	0.079	MS	
1280.6	49.147	2-Ethyl-3-methylmaleimide	0.094	MS	
1289.2	49.812	Anethole	0.065	MS, RI	Sweet, herbaceous, anise (artificial Licorice) odor
1291.0	49.958	Dihydroedulan I (trans)	0.060	MS, RI	
1294.8	50.250	2-Methylnaphthalene	0.000	MS, RI	Oily, aromatic, camphoraceous
1296.0	50.350	Dihydroedulan II (cis)	0.124	MS, RI	
1300.0	50.663	Tridecane	0.070	MS, RI	
1300.6	50.700	Theaspirane A ^a	trace	MS, RI	Weak camphoraceous
1307.0	51.124	3-Ethyl-4-methylpyrrolidindione	0.037	MS	
1310.4	51.350	Benzoic acid	trace	MS	Very weak, balsamic odor
1312.4	51.480	1-Methylnaphthalene	0.099	MS, RI	Green, musty, earthy, phenolic
1318.8	51.906	Theaspirane B ^a	0.035	MS, RI	Fruity, camphoraceous - naphthalene-like note
1329.6	52.637	Indole ^b	0.010	MS	Floral odor in dilution
1343.8	53.612	cis-5-Butyl-4-methyldihydrofuran-2(3H)-one (Oak lactone) ^a	0.024	MS	Coumarinic, coconut, lactonic, woody, maple and lovage
1353.7	54.300	Nonanoic acid	trace	MS	Fatty, musty, sweaty sour "goaty" notes
1366.5	55.211	Nicotine	30.246	MS	
1371.1	55.540	5-Pentyldihydrofuran-2(3H)-one; (gamma-nonalactone)	trace	MS, RI	Strong, fatty, coconut odor
1374.2	55.764	Solanone	0.962	MS	Smooth, ketonic
1385.3	56.567	1,1-Biphenyl	0.042	MS	
1390.9	56.977	Damascenone +unknown	0.240	MS, RI	Fruity-floral with apple-plum-raisin, tea, rose, tobacco notes
1393.5	57.170	1-Tetradecene	0.062	MS	

1397.3	57.450	2-Ethyl-naphthalene	trace	MS	
1400.0	57.651	Tetradecane	0.054	MS, RI	
1400.5	57.680	1-Ethyl-naphthalene	trace	MS	
1402.9	57.827	Vanillin	0.032	MS, RI	Sweet vanilla odor
1407.0	58.080	6,10-Dimethylundecan-2-one	trace	MS	Sweet herbaceous floral, fruity hay undernotes
1407.3	58.101	A Dimethylnaphthalene	0.039	MS	
1419.3	58.851	beta-Damascone	0.047	MS, RI	Tobacco, rose, tea, apple, fruity odor
1423.3	59.103	A Dimethylnaphthalene	0.026	MS	
1425.0	59.205	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)butan-2-one ^a	0.024	MS	
1427.3	59.350	A Dimethylnaphthalene + Myosmine	0.059	MS	
1432.8	59.700	alpha-Ionone	0.015	MS, RI	Woody, balsamic, violet odor; violet-raspberry in dilution
1441.8	60.280	Isoamyl benzoate	trace	MS	Sweet, balsamic, fruity
1443.1	60.360	A Dimethylnaphthalene	trace	MS	
1443.9	60.409	Dihydro-beta-ionone ^a	0.056	MS	Similar to beta-ionone, but weaker
1446.9	60.604	A Dimethylnaphthalene	0.011	MS	
1450.7	60.849	Acenaphthylene	0.026	MS	
1453.7	61.048	A Dimethylnaphthalene	0.012	MS	
1457.5	61.297	Geranylacetone	0.304	MS, RI	Fresh, floral, rosy-green-fruity odor
1460.7	61.502	Dimethyl phthalate	0.018	MS	
1463.5	61.684	9-oxo-Dihydroedulan I = (5S*,9R*)-3,4-dihydro-3-oxoedulan (cis isomer)	0.027	MS	Oriental tobacco, woody, ionone (mixed isomers)
1465.4	61.811	3-Phenylpyridine	0.019	MS	
1472.1	62.257	2,6-Di-tert-butylbenzoquinone ^a	0.025	MS	
1477.8	62.637	Nicotine-N-oxide	0.057	MS	
1482.0	62.915	gamma-Muurolene ^a	0.019	MS, RI	
1484.5	63.080	alpha-iso-Methylionone ^{a,b,c}	trace	MS	Sweet floral, violet-orris odor
1488.1	63.325	9-oxo-Dihydroedulan II = (5S*,9S*)-3,4-dihydro-3-oxoedulan (trans isomer)	0.063	MS	Oriental tobacco, woody, ionone (mixed isomers)
1488.4	63.345	Nicotyrine	0.138	MS	
1491.0	63.520	beta-Ionone + unknown	0.100	MS, RI	Woody, violet, fruity odor; woody-raspberry on dilution
1491.3	63.544	Phenethyl 2-methylbutanoate ^a	0.020	MS	Sweet fruity, herbaceous, floral odor
1494.7	63.770	Phenethyl isovalerate	0.024	MS, RI	Fruity, rose, balsamic odor
1496.9	63.920	A Methyl-1,1'-biphenyl	trace	MS	
1500.0	64.134	Pentadecane	0.052	MS, RI	
1505.0	64.432	alpha-Muurolene ^a	0.016	MS, RI	
1507.5	64.576	2-Isopropyl-naphthalene	0.017	MS	
1510.1	64.733	A Trimethylnaphthalene	trace	MS	
1512.1	64.850	Cuparene	trace	MS, RI	
1512.8	64.895	A Trimethylnaphthalene	trace	MS	

1516.2	65.096	9-oxo-Tetrahydroedulan I = (5S*,9S*)-3,4,6,7-Tetrahydro-3-oxoedulan (trans isomer)	0.054	MS	Sweet, floral, Burley tobacco, camphoraceous
1519.6	65.303	Dibenzofuran	0.021	MS	
1519.8	65.315	gamma-Cadinene	trace	MS, RI	
1525.7	65.665	A Trimethylnaphthalene	trace	MS	
1526.8	65.732	Methyl dodecanoate	trace	MS, RI	Weak waxy, creamy fatty
1529.2	65.878	delta-Cadinene	0.019	MS, RI	
1529.5	65.900	cis-Calamene	0.018	MS, RI	
1534.7	66.216	A Trimethylnaphthalene	0.002	MS	
1536.1	66.300	2,3-Dipyridyl	0.063	MS	
1539.0	66.478	Dihydroactinidiolide	0.112	MS	Sweet, floral osmanthus tea like aroma with a tobacco note odor
1551.0	67.214	A Trimethylnaphthalene	0.001	MS	
1551.3	67.234	A Trimethylnaphthalene	0.001	MS	
1553.9	67.391	A Trimethylnaphthalene	trace	MS	
1556.3	67.541	A Trimethylnaphthalene	trace	MS	
1566.2	68.160	A Trimethylnaphthalene	0.002	MS	
1568.2	68.282	(6Z,8E)-Megastigma-4,6,8-trien-3-one (Isomer I);	0.044	MS	Warm, Dry, Sweet, Tobacco-Like (mixed isomers)
1571.3	68.477	Dodecanoic acid	0.056	MS, RI	Weak, refreshing, fatty, waxy odor
1578.4	68.925	Gamma-Undecalactone ^a ; (5-Butyl-4-methyldihydrofuran-2(3H)-one)	0.009	MS	Strong fatty, Peach-Apricot odor
1578.8	68.955	Isoamyl salicylate	0.007	MS	Sweet, floral, herbaceous, green notes
1585.6	69.384	(6Z,8Z)-Megastigma-4,6,8-trien-3-one (Isomer II) + unknown	0.179	MS	Warm, Dry, Sweet, Tobacco-Like (mixed isomers)
1589.4	69.625	(E,E)-Pseudoionone	0.016	MS	
1593.2	69.869	1-Hexadecene	0.009	MS, RI	
1600.0	70.310	Hexadecane	0.013	MS, RI	
1602.3	70.439	Diethyl phthalate	0.503	MS	
1620.5	71.471	(6E,8E)-Megastigma-4,6,8-trien-3-one (Isomer III)	0.016	MS	Warm, Dry, Sweet, Tobacco-Like (mixed isomers)
1633.1	72.198	(6E,8Z)-Megastigma-4,6,8-trien-3-one (Isomer IV);	0.056	MS	Warm, Dry, Sweet, Tobacco-Like (mixed isomers)
1635.1	72.310	Benzophenone ^a	0.002	MS	Rose-like, geranium-like odor
1680.6	74.987	1-Tetradecanol	0.012	MS, RI	Weak oily fatty
1693.9	75.790	1-Heptadecene	0.000	MS	
1682.1	75.078	Hexyl salicylate ^a	0.001	MS	Dry, hay-like, waxy-balsamic floral odor
1700.0	76.162	Heptadecane	0.011	MS, RI	
1727.4	77.650	Methyl tetradecanoate ^a	0.002	MS, RI	Weak, fatty-cognac, oily-orris odor
1768.0	79.912	Tetradecanoic acid	0.054	MS, RI	Very faint, waxy-oily; nearly odorless
1784.7	80.860	Phenanthrene	trace	MS	
1793.1	81.340	1-Octadecene	trace	MS, RI	
1800.0	81.738	Octadecane	0.009	MS, RI	
1810.6	82.286	1,2-Diphenoxyethane ^a	0.013	MS	

1828.4	83.211	Isopropyl tetradecanoate ^a	0.006	MS	Faint, oily-fatty odor
1844.1	84.039	Neophtadiene	0.723	MS	
1848.5	84.274	6,10,14-Trimethyl-2-pentadecanone	0.009	MS, RI	Mild waxy, fresh oily, jasmine & celery note
1866.2	85.218	Pentadecanoic acid	0.020	MS, RI	
1877.4	85.824	Benzyl salicylate	0.002	MS	Sweet, floral, balsamic odor
1883.5	86.154	1-Hexadecanol	0.065	MS, RI	Faint waxy, nearly odorless
1900.0	87.052	Nonadecane	0.009	MS, RI	
1922.4	88.162	Farnesylacetone	0.007	MS, RI	Weak, floral, creamy, winey odor
1928.1	88.451	Methyl palmitate	0.004	MS, RI	Faint, waxy, sweet odor
1948.0	89.455	9-Hexadecenoic acid	0.037	MS, RI	Weak fatty-tallowy fried odor
1972.2	90.688	Dibutyl phthalate ^d + palmitic acid	0.766	MS, RI	Almost odorless
2000.0	92.128	n-Eicosane	0.004	MS, RI	
2026.9	93.405	Isopropyl palmitate ^a	0.008	MS	Nearly odorless
2087.7	96.358	1-Octadecanol	0.030	MS, RI	
2100.0	96.968	n-Heinecosane	0.007	MS, RI	
2129.3	98.303	Methyl stearate	0.002	MS, RI	Almost odorless
2143.9	98.977	Oleic acid (9-octadecenoic acid)	0.022	MS, RI	Weak fatty-tallowy fried odor
2151.9	99.347	Butyl isoamyl phthalate ^d	0.003	MS	
2167.5	100.070	Stearic acid	0.009	MS, RI	
2200.0	101.600	Docosane + butyl 2-methylbutyl phthalate ^d	0.004	MS, RI	
2300.0	106.041	Tricosane	0.006	MS, RI	
2328.0	107.222	Butyl 2-ethylhexylphthalate ^d	0.005	MS	
2358.9	108.538	Benzyl butyl phthalate ^d	0.004	MS	
2400.0	110.318	Tetracosane + unknown	0.010	MS, RI	
2500.0	114.114	Pentacosane + unknown	0.015	MS, RI	
2563.4	116.620	Di(2-ethylhexyl) phthalate ^d	0.011	MS	
2600.0	118.093	Hexacosane + unknown	0.961	MS, RI	
2700.0	122.860	Heptacosane	0.021	MS, RI	
2800.0	128.146	Octacosane	0.021	MS, RI	
2831.4	130.131	10-Demethylsqualene	0.093	MS	
2900.0	134.566	Nonacosane	0.021	MS, RI	
		Unidentified constituents	2.522		

^aNew tobacco isolate, ^bTentative identification, ^cPreviously found in Virginia tobacco by the authors, ^dPresumed to be an artifact from polyethylene storage bag

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CORRECTION - The material listed as 4-Hydroxy-4-methyl-2-butanone should read as 4-Hydroxy-4-methyl-2-pentanone (RI = 849.4)