

Date : 2023-07-11

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 23G04-PTH04

**Customer Identification :** Vetiver - India - V30110R

**Type :** Essential Oil

**Source :** *Vetiveria zizanioides* ct. *India* [syn. *Chrysopogon zizanioides* ct. *India*]

**Customer :** Plant Therapy

Checked and approved by:

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Alexis St-Gelais, Ph. D., Chimiste 2013-174

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## GAS CHROMATOGRAPHIC ANALYSIS

**Method :** PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID



**Results :** See analysis summary (next page)

**Analyst :** Sylvain Mercier, M. Sc., Chimiste 2014-005

**Date :** 2023-07-06

## PHYSICOCHEMICAL DATA

**Physical aspect :** Yellow/orange viscous liquid

**Analyst :** Cindy Caron B. Sc.

**Date :** 2023-07-05

**Refractive index :**  $1.5253 \pm 0.0003$  (20 °C)

**Method :** PC-MAT-016 - Measure of the refractive index of a liquid.

**Analyst :** Cindy Caron B. Sc.

**Date :** 2023-07-05

## CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

## ANALYSIS SUMMARY - CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
Isovaleral	tr	Aliphatic aldehyde
Furfural	0.01	Furan
Menthol	0.04	Monoterpenic alcohol
4-Vinylguaiacol	0.01	Simple phenolic
$\alpha$ -Cubebene	0.01	Sesquiterpene
Unknown	0.02	Norsesquiterpene
Cyclosativene I	0.06	Sesquiterpene
12-Norisoziza-5-ene	0.05	Norsesquiterpene
$\alpha$ -Ylangene	0.12	Sesquiterpene
2-Norzizaene?	0.12	Norsesquiterpene
6-epi-Nigritene	0.08	Norsesquiterpene
Nigritene	0.15	Norsesquiterpene
$\beta$ -Elemene	0.04	Sesquiterpene
Cyperene	0.02	Sesquiterpene
Acora-3,7(14)-diene	0.15	Sesquiterpene
$\alpha$ -Cedrene	0.16	Sesquiterpene
$\beta$ -Caryophyllene	0.08	Sesquiterpene
Cascarilladiene	0.06	Sesquiterpene
$\beta$ -Cedrene	0.14	Sesquiterpene
Unknown	0.19	Sesquiterpene
6,9-Guaiadiene	0.14	Sesquiterpene
Prezizaene	0.73	Sesquiterpene
Khusimene	0.72	Sesquiterpene
Selina-4(15),7-diene	0.30	Sesquiterpene
Unknown	0.08	Sesquiterpene
Unknown	0.28	Sesquiterpene
Unknown	0.32	Sesquiterpene
$\alpha$ -Amorphene	1.79	Sesquiterpene
Unknown	0.46	Unknown
$\alpha$ -Vetispirene	0.60	Sesquiterpene
$\beta$ -Vetispirene	1.74	Sesquiterpene
Bicyclosesquiphellandrene?	0.59	Sesquiterpene
Eudesma-2,4(15),11-triene	0.38	Sesquiterpene
$\delta$ -Amorphene	1.21	Sesquiterpene
$\gamma$ -Cadinene	0.41	Sesquiterpene
Nootkatene	0.12	Sesquiterpene
Spirovettiva-1(10),7(11)-diene	0.72	Sesquiterpene
$\delta$ -Cadinene	0.13	Sesquiterpene
trans-Calamenene	0.03	Sesquiterpene
$\gamma$ -Vetivenene	0.77	Sesquiterpene

$\alpha$ -Calacorene	0.38	Sesquiterpene
$\beta$ -Vetivenene	4.88	Sesquiterpene
$\alpha$ -Elemol	0.16	Sesquiterpenic alcohol
Unknown	0.36	Sesquiterpene
Eremophila-1(10),11-dien-9 $\beta$ -ol	0.46	Sesquiterpenic alcohol
cis-Eudesm-6-en-11-ol	1.20	Sesquiterpenic alcohol
Unknown	0.14	Oxygenated sesquiterpene
Gynuradienol?	0.39	Sesquiterpenic alcohol
Unknown	1.00	Sesquiterpene
Unknown	0.33	Sesquiterpene
Unknown	0.34	Oxygenated sesquiterpene
Khusimone	0.62	Norsesquiterpenic ketone
Eudesm-4-en-7 $\alpha$ -ol	0.20	Sesquiterpenic alcohol
Unknown	0.88	Sesquiterpene
10-epi- $\gamma$ -Eudesmol	0.36	Sesquiterpenic alcohol
Selin-6-en-4 $\alpha$ -ol isomer	1.29	Sesquiterpenic alcohol
Selin-6-en-4 $\alpha$ -ol	0.61	Sesquiterpenic alcohol
Unknown	0.57	Oxygenated sesquiterpene
Unknown	1.14	Unknown
Unknown	1.16	Oxygenated sesquiterpene
Unknown	1.42	Oxygenated sesquiterpene
Cyclocopacamphan-12-ol, epimer A	1.13	Sesquiterpenic alcohol
Unknown	2.15	Sesquiterpenic alcohol
Unknown	0.86	Oxygenated sesquiterpene
Cyclocopacamphan-12-ol, epimer B	1.65	Sesquiterpenic alcohol
Unknown	1.21	Oxygenated sesquiterpene
Khusinol	0.31	Sesquiterpenic alcohol
Zizanol	1.58	Sesquiterpenic alcohol
Zizanone analog	0.26	Sesquiterpenic ketone
Khusiol	1.17	Sesquiterpenic alcohol
epi-Zizanone	0.76	Sesquiterpenic ketone
Zizanal	0.96	Sesquiterpenic aldehyde
Unknown	1.56	Oxygenated sesquiterpene
Juniper camphor	0.66	Sesquiterpenic alcohol
Unknown	0.76	Oxygenated sesquiterpene
Unknown	0.35	Oxygenated sesquiterpene
Vetiselinol	2.29	Sesquiterpenic alcohol
$\alpha$ -Vetivol?	0.34	Sesquiterpenic alcohol
Unknown	0.22	Oxygenated sesquiterpene
Khusimol	10.18	Sesquiterpenic alcohol
Unknown	2.03	Oxygenated sesquiterpene
10-epi-Acora-3,11-dien-15-al?	1.02	Sesquiterpenic aldehyde
Unknown	0.27	Oxygenated sesquiterpene
Unknown	0.30	Unknown
(E)-Isovalencenol	6.14	Sesquiterpenic alcohol

Unknown	1.04	Oxygenated sesquiterpene
Nootkatone	0.66	Sesquiterpenic ketone
Unknown	0.10	Oxygenated sesquiterpene
(Z)-Isovalencenal	1.04	Sesquiterpenic aldehyde
$\beta$ -Vetivone	1.81	Sesquiterpenic ketone
(E)-Isovalencenal	2.21	Sesquiterpenic aldehyde
Zizanoic acid	5.50	Sesquiterpenic acid
$\alpha$ -Vetivone	2.67	Sesquiterpenic ketone
Unknown	0.61	Oxygenated sesquiterpene
Isovalencenal isomer II?	0.30	Sesquiterpenic aldehyde
Isovalencenal isomer I?	0.20	Sesquiterpenic aldehyde
$\beta$ -Cyclodihydrocostunolide?	0.11	Sesquiterpenic lactone
<b>Consolidated total</b>	<b>85.29</b>	

tr: The compound has been detected below 0.005% of the total signal

Note: no correction factor was applied

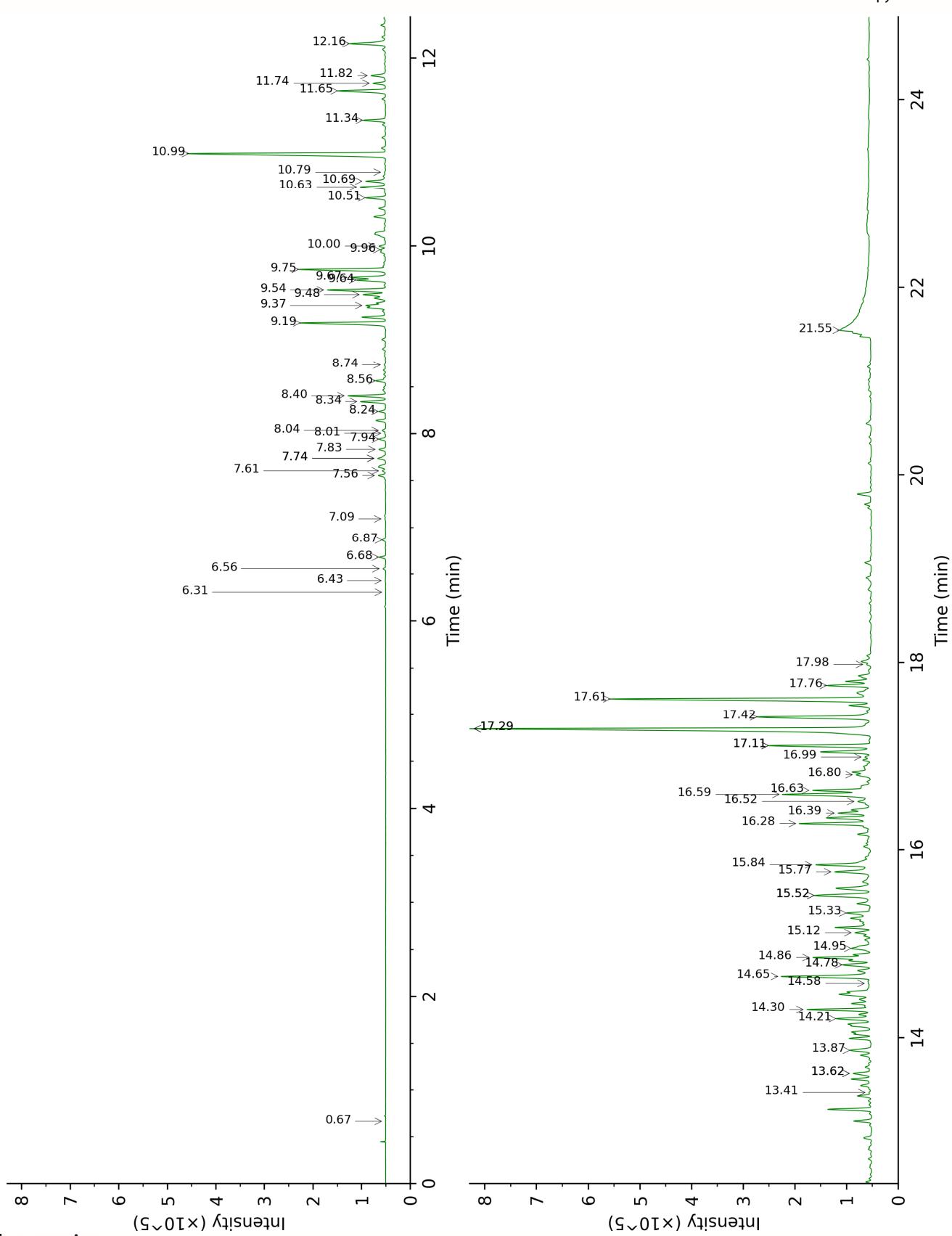
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm is set to prioritize data from the most standard DB-5 column, and smallest values so as to avoid overestimating individual content. This process is semi-automatic. Advanced users are invited to consult the "Full analysis data" table after the chromatograms in this report to access the full untreated data and perform their own calculations if needed.

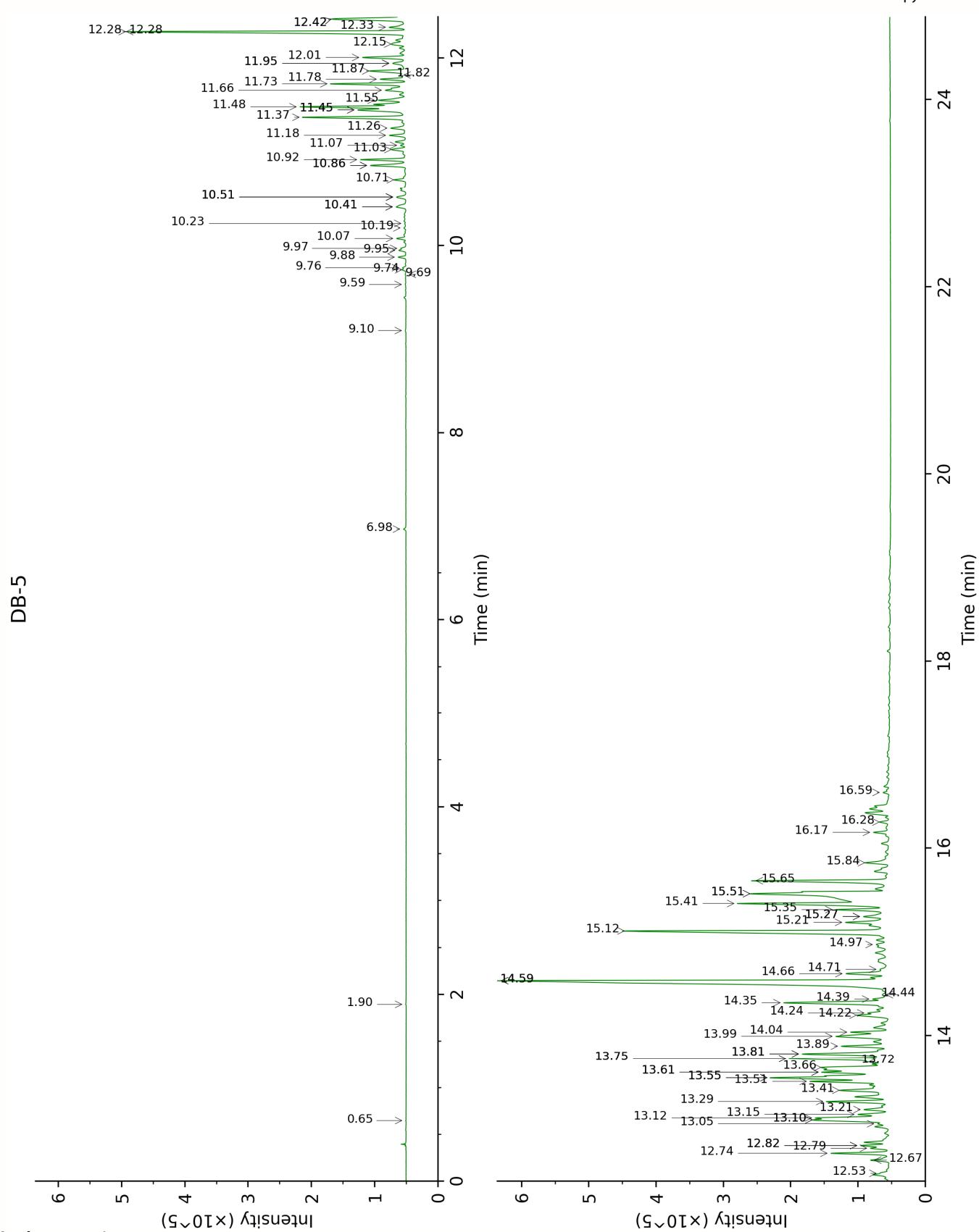
**Unknowns:** Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

**Bracketed value ([xx]):** A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

This page was intentionally left blank. The following pages present the complete data of the analysis.

DB-WAX





**FULL ANALYSIS DATA**

<b>Isovaleral</b>	<b>Column DB-WAX</b>			<b>Column DB-5</b>		
	0.67	884.0	tr	0.65	641.1	tr
Furfural	6.31	1412.6	0.01	1.90	830.8	0.01
Menthol	8.74	1599.1	0.04	6.98	1171.8	0.04
4-Vinylguaiacol	14.58	2125.1	0.06	9.10	1312.2	0.01
$\alpha$ -Cubebene	6.43	1421.8	0.01	9.59	1346.6	0.01
Unknown CHZI VIII [m/z 145, 188 (95), 117 (91), 173 (80), 91 (65), 131 (64)]				9.69	1354.2	0.02
Cyclosativene I	6.56	1431.3	0.05	9.74	1357.6	0.06
12-Norisoziza-5-ene	6.87	1454.5	0.07	9.76	1359.2	0.05
$\alpha$ -Ylangene	6.68	1440.6	0.12	9.88	1367.1	0.12
2-Norzaene?				9.95	1372.2	0.12
6-epi-Nigritene	7.61	1510.3	0.07	9.97	1373.6	0.08
Nigritene	7.74*	1520.7	[0.21]	10.08	1381.1	0.15
$\beta$ -Elemene	8.01	1541.7	0.02	10.19	1388.9	0.04
Cyperene	7.10	1471.7	0.02	10.23	1392.3	0.02
Acora-3,7(14)-diene	7.84	1528.2	0.15	10.41*	1404.7	[0.25]
$\alpha$ -Cedrene	7.56	1506.5	0.16	10.41*	1404.7	[0.25]
$\beta$ -Caryophyllene	8.04	1544.1	0.08	10.51*	1412.4	[0.19]
Cascarilladiene	7.74*	1520.7	[0.21]	10.51*	1412.4	[0.19]
$\beta$ -Cedrene	7.94	1536.8	0.14	10.51*	1412.4	[0.19]
Unknown POBA XXIV [m/z 161, 105 (35), 119 (23), 93 (16), 91 (16), 81 (15)... 204 (3)]				10.70	1426.6	0.19
6,9-Guaiadiene	8.24	1560.0	0.14	10.86*	1438.0	[0.68]
Prezizaene	8.40	1573.1	0.73	10.86*	1438.0	[0.68]
Khusimene	8.34	1568.2	0.50	10.92	1442.6	0.72
Selina-4(15),7-diene	8.56	1585.7	0.20	11.03	1450.6	0.30
Unknown CHZI X [m/z 119, 190 (99), 175 (95), 105 (71), 91 (59), 120 (57)... 204 (2)]				11.07	1453.9	0.08
Unknown CHZI XI [m/z 119, 120 (31), 83 (23), 105 (22), 91 (21), 81 (18)... 202 (9)]	9.37	1650.9	0.39	11.18	1461.9	0.29
Unknown CHZI XII [m/z 145, 202 (85), 159 (64), 187 (39), 131 (35), 117 (34)]	9.48	1660.4	0.49	11.26	1467.6	0.32
$\alpha$ -Amorphene	9.19	1635.7	1.82	11.37	1476.2	1.79
Unknown MISC CLXXI [m/z 160, 145 (78), 91 (37), 108 (31), 105 (28)...]				11.45*	1482.0	[1.05]
$\alpha$ -Vetispirene	9.64	1673.2	0.60	11.45*	1482.0	[1.05]

Essential Oil, *Vetiveria zizanioides* ct. India [syn. *Chrysopogon zizanioides* ct. India]  
Internal code: 23G04-PTH04

Vetiver - India - V30110R

Plant Therapy

$\beta$ -Vetispirene	9.75	1682.4	1.77	11.48	1484.5	1.74
Bicyclosesquiphellandrene?				11.55	1489.7	0.59
Eudesma-2,4(15),11-triene	10.69	1762.3	0.46	11.66	1497.7	0.38
$\delta$ -Amorphene	9.54	1664.5	1.28	11.73	1502.8	1.21
$\gamma$ -Cadinene	9.96	1699.6	0.10	11.78	1506.5	0.41
Nootkatene	10.51	1746.7	0.40	11.82	1509.9	0.12
Spirovetiva-1(10),7(11)-diene	9.67	1675.4	0.71	11.86	1513.3	0.72
$\delta$ -Cadinene	10.00	1702.8	0.13	11.95*	1519.7	[0.37]
<i>trans</i> -Calamenene	10.79	1770.7	0.03	11.95*	1519.7	[0.37]
$\gamma$ -Vetivenene	10.63	1756.9	0.52	12.01	1524.6	0.77
$\alpha$ -Calacorene	11.74	1854.2	0.25	12.15	1535.8	0.38
$\beta$ -Vetivenene	10.99	1787.8	4.88	12.28*	1546.2	[5.04]
$\alpha$ -Elemol	13.62*	2029.7	[0.51]	12.28*	1546.2	[5.04]
Unknown CHZI XLIII [m/z 200, 185 (82), 143 (54), 157 (36), 123 (34), 128 (32)...]				12.33	1549.9	0.36
Eremophila-1(10),11-dien-9 $\beta$ -ol	11.34	1818.7	0.46	12.42*	1556.8	[1.65]
<i>cis</i> -Eudesm-6-en-11-ol				12.42*	1556.8	[1.65]
Unknown CHZI XIII [m/z 81, 200 (55), 143 (36), 93 (33), 91 (32), 185 (31), 129 (27), 128 (21)...]				12.52	1565.1	0.14
Gynuradienol?	13.87	2054.7	0.61	12.67	1576.2	0.39
Unknown CHZI V [m/z 202, 187 (63), 145 (43), 159 (34), 131 (29), 91 (22), 117 (20)]	11.66	1846.9	1.06	12.74	1582.0	1.00
Unknown CHZI XLIV [m/z 162, 119 (83), 43 (60), 147 (53), 91 (36), 204 (32)]				12.79	1586.2	0.33
Unknown POBA V [m/z 161, 119 (78), 105 (75), 120 (72), 43 (64)... 218 (4)]	11.82	1861.6	0.34	12.82*†	1588.4	[0.50]
Khusimone				12.82*†	1588.4	[0.50]
Eudesm-4-en-7 $\alpha$ -ol	13.41	2009.8	0.06	13.05	1606.7	0.20
Unknown CHZI VI [m/z 187, 202 (86), 145 (25), 131 (19), 105 (16), 188 (15)]	12.16	1892.2	0.88	13.10*†	1610.2	[1.61]
10-epi- $\gamma$ -Eudesmol	13.62*	2029.7	[0.51]	13.10*†	1610.2	[1.61]
Selin-6-en-4 $\alpha$ -ol isomer	14.30	2097.3	1.29	13.12*†	1611.8	[1.23]
Selin-6-en-4 $\alpha$ -ol	15.12	2180.6	0.41	13.15	1615.0	0.61
Unknown CHZI XXVIII [m/z 59, 149 (94), 43 (82), 205 (65)... 220 (6)]				13.21	1619.2	0.57

Unknown CHZI XXV [m/z 145, 59 (97), 161 (87), 218 (76), 43 (76), 179 (63)...]			13.29	1626.3	1.14	
Unknown CASA XXIX [m/z 187, 93 (35), 81 (34), 79 (31), 41 (30), 91 (30), 107 (29)... 220 (4)]	14.95	2163.4	0.80	13.41	1636.2	1.16
Unknown CHZI II [m/z 121, 107 (69), 93 (64), 79 (60), 177 (59), 136 (58), 91 (57), 41 (56)... 220 (21)]	14.86	2153.5	1.23	13.51	1644.1	1.42
Cyclocopacamphan-12-ol, epimer A	15.77	2248.5	1.13	13.55*†	1647.3	[2.54]
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	14.65	2132.8	2.15	13.55*†	1647.3	[2.54]
Unknown CHZI XV [m/z 161, 59 (67), 95 (45), 93 (40), 105 (40), 149 (39), 81 (39), 43 (38), 204 (37)... 220 (5)]	14.21	2087.8	0.86	13.60*†	1652.2	[1.23]
Cyclocopacamphan-12-ol, epimer B	15.84	2256.5	1.65	13.60*†	1652.2	[1.23]
Unknown CHZI XXVII [m/z 84, 119 (77), 41 (72), 81 (68), 95 (68), 93 (68), 109 (63)... 222 (17)]				13.66*†	1656.4	[1.48]
Khusinol	15.33	2202.2	0.66	13.72	1661.8	0.31
Zizanol	16.28	2303.4	1.58	13.75*	1664.4	[1.83]
Zizanone analog				13.75*	1664.4	[1.83]
Khusiol	15.52*	2221.6	[1.68]	13.81*	1668.8	[1.93]
epi-Zizanone	14.78	2145.5	0.76	13.81*	1668.8	[1.93]
Zizanal	16.63	2342.2	1.45	13.89	1675.7	0.96
Unknown CHZI XXVI [m/z 189, 43 (91), 81 (89), 105 (81), 91 (74), 93 (74), 133 (67), 41 (67)... 222 (37)]				13.99	1684.3	1.56
Juniper camphor	15.52*	2221.6	[1.68]	14.04	1688.0	0.66
Unknown CHZI I [m/z 189, 159 (82), 133 (44), 91 (29), 105 (29), 205 (25)... 220 (13)]	16.39	2315.4	0.80	14.22	1703.0	0.76
Unknown CHZI XIX [m/z 204, 189 (99), 43 (83), 161 (75), 105 (55), 91 (44), 119				14.24	1704.9	0.35

(33)... 220 (13)]						
Vetiselinol	16.59	2337.4	2.25	14.35	1714.3	2.29
α-Vetivol?	17.11*	2395.1	[2.15]	14.39	1717.7	0.34
Unknown CHZI XX [m/z 136, 121 (98), 137 (90), 119 (68), 107 (55), 135 (55)... 202 (30), 220 (27)]	16.80	2360.6	0.44	14.44	1721.7	0.21
Khusimol	17.29*	2415.1	[10.83]	14.59*	1734.7	[12.20]
Unknown CHZI XXIII [m/z 189, 187 (29), 159 (23), 43 (20), 133 (16)...]				14.59*	1734.7	[12.20]
10-epi-Acora-3,11-dien-15-al?				14.66	1741.2	1.02
Unknown CAIN XLIII [m/z 91, 105 (89), 79 (84), 93 (77), 107 (67), 189 (64), 145 (62), 119 (61)... 220 (16)...]				14.71	1745.1	0.27
Unknown CHZI XXXVIII [m/z 174, 131 (37), 159 (25), 91 (20), 175 (14)...]	16.99	2381.6	0.15	14.97	1768.0	0.30
(E)-Isovalencenol	17.61	2452.3	6.03	15.12	1780.6	6.14
Unknown CHZI VII [m/z 120, 121 (93), 93 (85), 105 (74), 119 (68), 91 (58), 123 (49)... 220 (8)]	17.76	2468.8	0.97	15.21	1788.5	1.04
Nootkatone	17.29*	2415.1	[10.83]	15.27*	1793.9	[0.76]
Unknown CHZI XXI [m/z 202, 187 (91), 93 (70), 91 (69), 105 (67)...]	17.98	2494.7	0.10	15.27*	1793.9	[0.76]
(Z)-Isovalencenal	16.52	2329.0	0.44	15.34	1800.3	1.04
β-Vetivone	17.11*	2395.1	[2.15]	15.41*†	1805.9	[3.23]
(E)-Isovalencenal				15.51*†	1815.4	[6.28]
Zizanoic acid	21.55	2943.4	5.49	15.51*†	1815.4	[6.28]
α-Vetivone	17.42	2429.6	2.82	15.65	1828.0	2.67
Unknown CHZI XXIX [m/z 105, 179 (87), 91 (67), 161 (61), 121 (57), 119 (56), 163 (50), 43 (50)...]				15.84	1845.4	0.61
Isovalencenal isomer II?				16.17	1874.9	0.30
Isovalencenal isomer I?				16.28	1884.9	0.20
β-Cyclodihydrocostunolide?				16.59	1913.8	0.11
Total reported		68.66%			85.49%	

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is taken into account in the consolidated total

†: Peaks apexes were resolved, but peaks overlapped and were summed for analysis

tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index