

Date : 2024-06-26

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24F11-PTH01

Customer Identification : Vetiver - Indonesia - Lot: V30111R

Type : Essential Oil

Source : *Chrysopogon zizanioides* ct. Indonesia

Customer : Plant Therapy

Checked and approved by:

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 liquide by FAST GC-FID

***ISO**

Results : See analysis summary (next page)

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

Date : 2024-06-17

PHYSICOCHEMICAL DATA

Refractive index : 1.5254 ± 0.0003 (20 °C)

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

Analyst : Cindy Caron B. Sc.

Date : 2024-06-14

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	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Furfural	0.25	Furan
α -Pinene	0.01	Monoterpene
5-Methylfurfural	0.02	Furan
2-Furfurylfuran	0.02	Furan
<i>ortho</i> -Guaiacol	0.03	Simple phenolic
4-Ethylguaiacol	0.04	Norphenylpropanoid
4-Vinylguaiacol	0.13	Simple phenolic
Unknown	0.12	Sesquiterpene
2-Norprezizene	0.09	Sesquiterpene
Unknown	0.17	Unknown
Eugenol	0.02	Phenylpropanoid
12-Norisoziza-5-ene	1.13	Norsesquiterpene
Unknown	0.38	Norsesquiterpene
α -Ylangene	0.11	Sesquiterpene
α -Copaene	0.01	Sesquiterpene
6- <i>epi</i> -Nigritene	1.30	Norsesquiterpene
Nigritene	2.12	Norsesquiterpene
Unknown	0.19	Unknown
Acora-3,7(14)-diene	0.27	Sesquiterpene
Isoeugenol isomer	0.15	Phenylpropanoid
β -Cedrene	0.30	Sesquiterpene
Unknown	0.51	Sesquiterpene
β -Copaene	0.05	Sesquiterpene
Unknown	0.35	Sesquiterpene
Prezizaene	0.69	Sesquiterpene
Unknown	1.30	Norsesquiterpene
Khusimene	1.05	Sesquiterpene
(<i>E</i>)-Isoeugenol	0.52	Phenylpropanoid
Selina-4(15),7-diene	0.44	Sesquiterpene
Unknown	0.40	Sesquiterpene
Unknown	0.51	Sesquiterpene
Unknown	0.62	Sesquiterpene
α -Amorphene	2.14	Sesquiterpene
α -Vetispirene	1.88	Sesquiterpene
<i>cis</i> -Eudesma-6,11-diene	1.48	Sesquiterpene
β -Vetispirene	2.01	Sesquiterpene
γ -Amorphene	0.18	Sesquiterpene
δ -Selinene	1.20	Sesquiterpene

Bicyclosquiphellandrene?	0.79	Sesquiterpene
Unknown	0.25	Sesquiterpene
δ-Amorphene	1.42	Sesquiterpene
Nootkatene	0.63	Sesquiterpene
β-Curcumene	0.15	Sesquiterpene
Spirovetiva-1(10),7(11)-diene	1.03	Sesquiterpene
Sesquicineole	0.06	Sesquiterpenic ether
trans-Calamenene	0.08	Sesquiterpene
δ-Cadinene	0.52	Sesquiterpene
γ-Vetivenene	2.99	Sesquiterpene
Selina-4(15),7(11)-diene	0.43	Sesquiterpene
Selina-4,7(11)-diene?	0.35	Sesquiterpene
α-Calacorene	0.66	Sesquiterpene
α-Elemol	0.34	Sesquiterpenic alcohol
β-Vetivenene	6.48	Sesquiterpene
Unknown	0.30	Sesquiterpene
Eudesma-5,7(11)-diene	0.50	Sesquiterpene
Eremophila-1(10),11-dien-9β-ol	2.12	Sesquiterpenic alcohol
Unknown	0.16	Oxygenated sesquiterpene
Unknown	1.31	Sesquiterpene
Khusimone	0.41	Norsesquiterpenic ketone
β-Oplophenone?	0.16	Sesquiterpenic ketone
Unknown	0.21	Oxygenated sesquiterpene
Junenol	0.33	Sesquiterpenic alcohol
Unknown	1.59	Sesquiterpene
Selin-6-en-4α-ol	0.11	Sesquiterpenic alcohol
Unknown	0.62	Unknown
Unknown	1.03	Oxygenated sesquiterpene
τ-Cadinol	0.76	Sesquiterpenic alcohol
Unknown	1.17	Oxygenated sesquiterpene
Unknown	0.38	Oxygenated sesquiterpene
Unknown	0.56	Sesquiterpenic alcohol
Cyclocopacamphan-12-ol, epimer A	0.79	Sesquiterpenic alcohol
Cyclocopacamphan-12-ol, epimer B	1.42	Sesquiterpenic alcohol
Zizanone analog	0.39	Sesquiterpenic ketone
Zizanol	1.48	Sesquiterpenic alcohol
Khusiol	1.45	Sesquiterpenic alcohol
epi-Zizanone	0.22	Sesquiterpenic ketone
Zizanal	0.76	Sesquiterpenic aldehyde
Unknown	1.27	Oxygenated sesquiterpene
Unknown	3.36	Oxygenated sesquiterpene
Vetiselinenol	1.74	Sesquiterpenic alcohol
Khusimol	5.91	Sesquiterpenic alcohol
Unknown	0.30	Oxygenated sesquiterpene
10-epi-Acora-3,11-dien-15-al?	0.72	Sesquiterpenic aldehyde

γ-Costol	0.12	Sesquiterpenic alcohol
Unknown	0.25	Unknown
13-Hydroxyvalencene?	0.35	Sesquiterpenic alcohol
(E)-Isovalencenol	1.22	Sesquiterpenic alcohol
Isozizanoic acid	2.80	Sesquiterpenic acid
Unknown	0.26	Oxygenated sesquiterpene
Nootkatone	0.25	Sesquiterpenic ketone
(Z)-Isovalencenal	0.91	Sesquiterpenic aldehyde
β-Vetivone	1.96	Sesquiterpenic ketone
Zizanoic acid	4.01	Sesquiterpenic acid
(E)-Isovalencenal	0.51	Sesquiterpenic aldehyde
Unknown	0.34	Unknown
α-Vetivone	2.07	Sesquiterpenic ketone
(E)-Eremophila-1(10),7(11)-dien-12-yl acetate	0.29	Sesquiterpenic ester
(E)-Isovalencenyl acetate?	0.07	Sesquiterpenic ester
Isovalencenal isomer I?	0.08	Sesquiterpenic aldehyde
β-Cyclodihydrocostunolide?	0.11	Sesquiterpenic lactone
Cembrene?	0.17	Diterpene
Consolidated total	85.69	

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

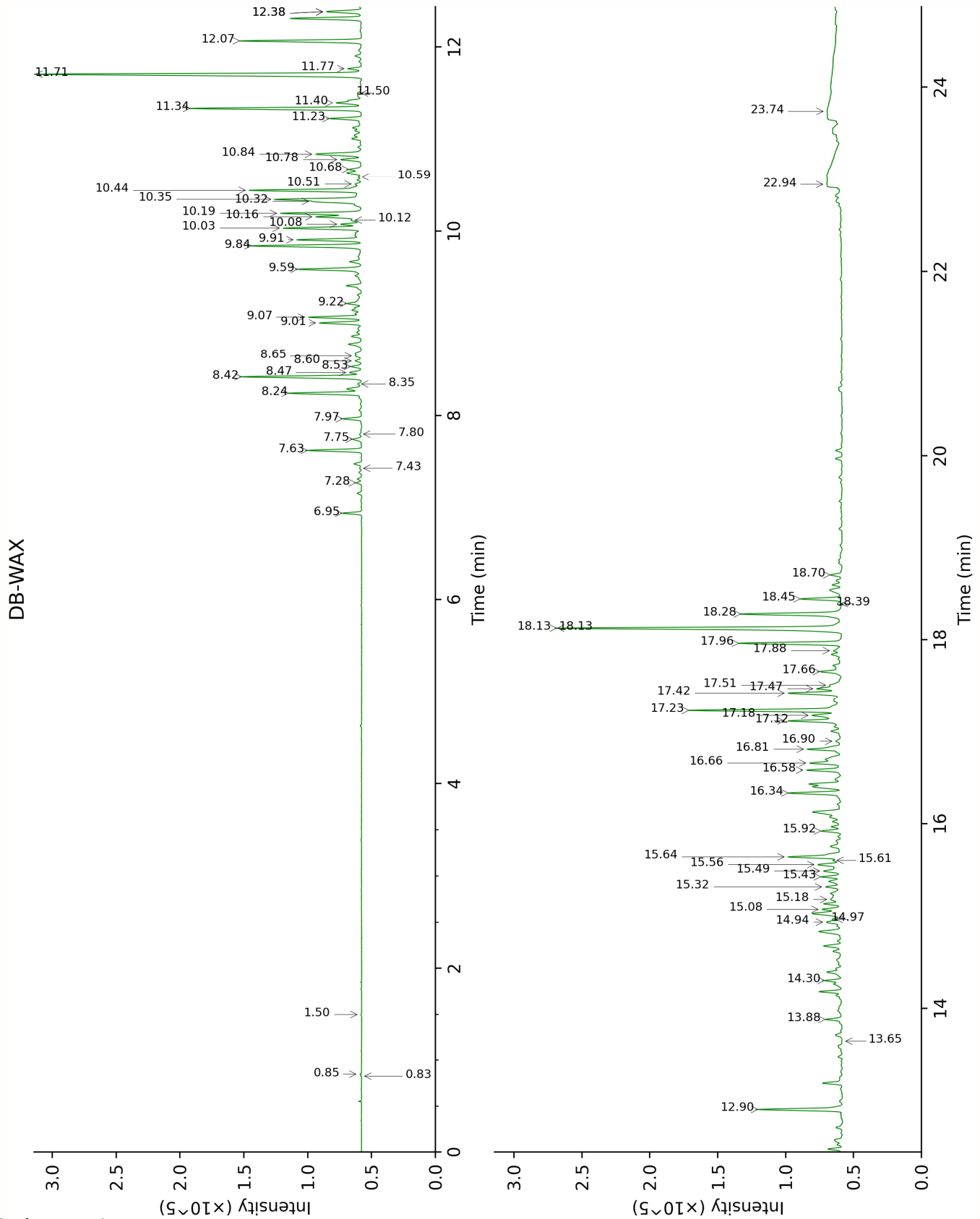
Note: no correction factor was applied

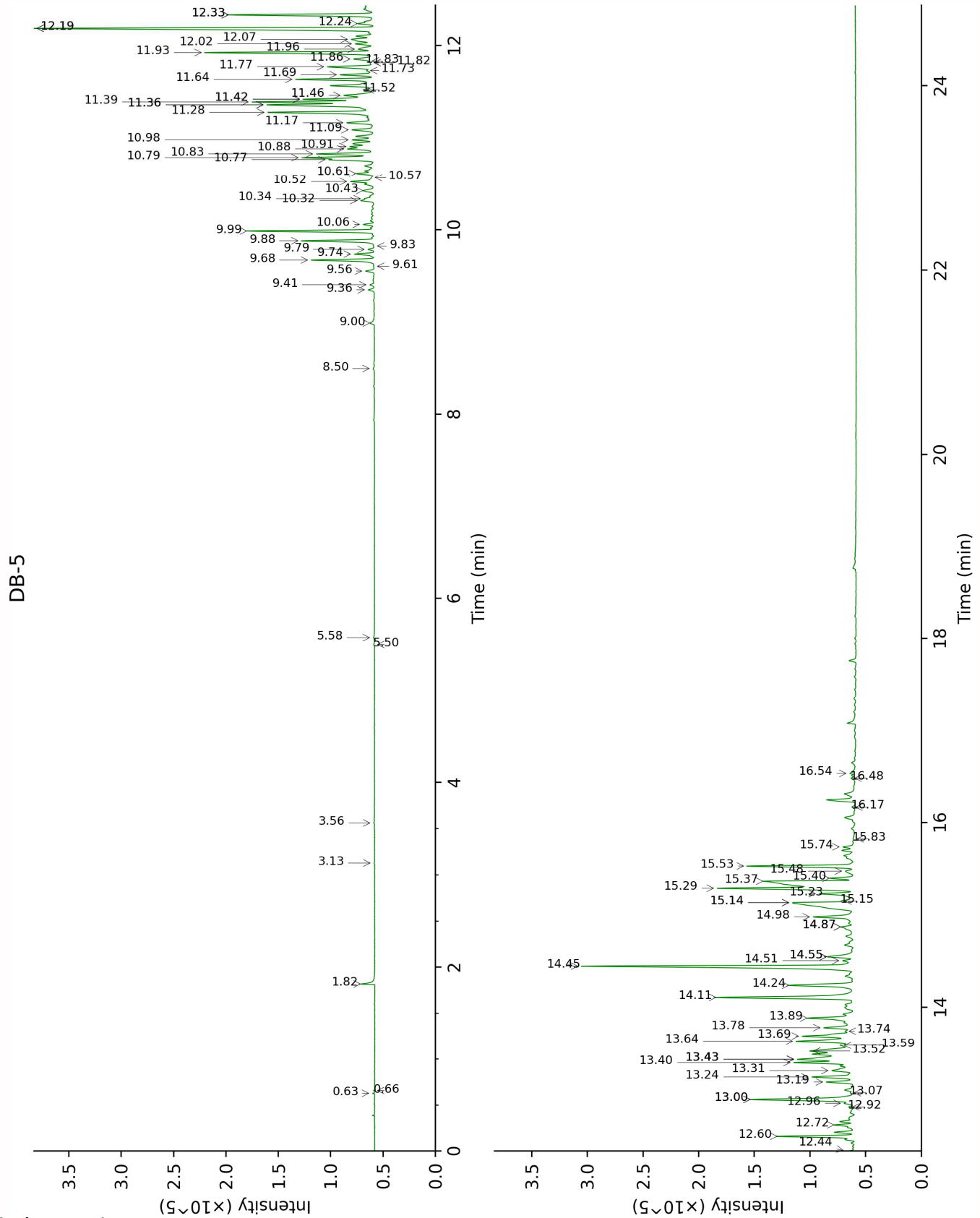
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.





FULL ANALYSIS DATA

Isovaleral	Column DB-WAX			Column DB-5		
	0.85	884.8	0.01	0.63	640.9	0.01
2-Methylbutyral	0.83	877.2	0.01	0.66	651.3	0.01
Furfural	6.95	1412.9	0.31	1.82	829.1	0.25
α -Pinene	1.50	990.3	0.01	3.13	931.0	0.01
5-Methylfurfural	8.34	1517.3	0.08	3.56	959.7	0.02
2-Furfurylfuran				5.50	1083.8	0.02
<i>ortho</i> -Guaiacol	11.77	1793.6	0.24	5.58	1088.4	0.03
4-Ethylguaiacol	13.65	1961.2	0.02	8.50	1278.2	0.04
4-Vinylguaiacol	15.43	2130.7	0.41	9.00	1312.0	0.13
Unknown CHZI XXXV [m/z 120, 91 (31), 92 (23), 121 (10), 105 (9), 119 (6)...202 (1)]				9.36	1337.3	0.12
2-Norprezizene	7.80	1476.1	0.04	9.41	1341.2	0.09
Unknown CHZI XXXIV [m/z 119, 91 (23), 120 (17), 118 (11), 92 (7), 105 (6)...]	7.75	1472.1	0.20	9.56	1351.6	0.17
Eugenol	15.08	2096.1	0.42	9.61	1355.2	0.02
12-Norisoziza-5-ene	7.63	1463.1	0.97	9.68	1360.0	1.13
Unknown CHZI III [m/z 119, 147 (85), 161 (75), 91 (69), 105 (62), 134 (60), 190 (43)]	7.97	1488.4	0.34	9.74	1364.5	0.38
α -Ylangene	7.28	1437.2	0.10	9.79	1368.1	0.11
α -Copaene	7.43	1448.9	0.05	9.83	1370.7	0.01
6-epi-Nigritene	8.24	1509.6	1.40	9.88	1374.6	1.30
Nigritene	8.42	1523.3	2.27	9.99	1382.1	2.12
Unknown CHZI XXXVI [m/z 119, 91 (24), 120 (17), 118 (10), 92 (8), 41 (7), 105 (6)...]	8.53	1531.9	0.21	10.06	1387.1	0.19
Acora-3,7(14)-diene	8.47	1526.8	0.26	10.32	1405.4	0.27
Isoeugenol isomer				10.34	1406.8	0.15
β -Cedrene	8.60	1536.6	0.13	10.42	1413.4	0.30
Unknown CHZI XLVI [m/z 132, 117 (71), 131 (19), 91 (16), 115 (15)... 202 (10)]				10.52	1420.7	0.51
β -Copaene	8.65	1540.8	0.12	10.57	1423.9	0.05
Unknown POBA XXIV [m/z 161, 105 (35), 119 (23), 93 (16), 91 (16), 81 (15)... 204 (3)]				10.61	1427.5	0.35
Prezizaene	9.01	1568.7	0.81	10.77	1438.8	0.69
Unknown CHZI IV [m/z 175, 190 (73), 161 (65), 119 (40),	9.59	1614.2	1.29	10.79	1440.4	1.30

105 (35), 91 (28), 133 (23)]						
Khusimene	9.07	1573.4	1.00	10.83	1443.4	1.05
(E)-Isoeugenol	16.81	2269.9	0.86	10.88	1447.5	0.52
Selina-4(15),7-diene	9.22	1584.7	0.42	10.91	1449.4	0.44
Unknown CHZI X [m/z 119, 190 (99), 175 (95), 105 (71), 91 (59), 120 (57)... 204 (2)]				10.98	1454.8	0.40
Unknown CHZI XI [m/z 119, 120 (31), 83 (23), 105 (22), 91 (21), 81 (18)... 202 (9)]	10.08	1653.2	0.36	11.09	1462.9	0.51
Unknown CHZI XII [m/z 145, 202 (85), 159 (64), 187 (39), 131 (35), 117 (34)]	10.16	1659.6	0.89	11.17	1468.6	0.62
α -Amorphene	9.84	1634.5	2.12	11.28	1477.0	2.14
α -Vetispirene	10.34	1674.7	1.88	11.36*	1483.0	[2.41]
<i>cis</i> -Eudesma-6,11-diene	10.03	1649.8	1.48	11.36*	1483.0	[2.41]
β -Vetispirene	10.44	1682.6	2.23	11.39	1485.3	2.01
γ -Amorphene	10.12	1656.7	0.18	11.42*	1487.6	[1.33]
δ -Selinene	9.91	1639.7	1.20	11.42*	1487.6	[1.33]
Bicyclosesquiphellandrene?				11.46	1490.7	0.79
Unknown CHZI XLII [m/z 119, 131 (43), 120 (38), 83 (38), 202 (31)]				11.52	1495.2	0.25
δ -Amorphene	10.19	1662.6	1.52	11.64	1503.6	1.42
Nootkatene	11.23	1748.1	0.58	11.69	1507.5	0.63
β -Curcumene	10.51	1688.0	0.12	11.73	1511.0	0.15
Spirovetiva-1(10),7(11)-diene	10.32	1673.0	0.61	11.77	1514.2	1.03
Sesquicineole	10.59	1694.6	0.06	11.82	1517.7	0.06
<i>trans</i> -Calamenene	11.50	1771.1	0.07	11.83	1519.1	0.08
δ -Cadinene	10.68	1701.8	0.24	11.86	1520.8	0.52
γ -Vetivenene	11.34	1757.3	3.17	11.93	1526.3	2.99
Selina-4(15),7(11)-diene	10.84	1715.7	1.10	11.96	1529.2	0.43
Selina-4,7(11)-diene?	10.78	1710.8	0.41	12.02	1533.7	0.35
α -Calacorene	12.38*	1847.7	[0.73]	12.07	1537.5	0.66
α -Elemol	14.30	2022.5	0.34	12.19*	1546.9	[6.29]
β -Vetivenene	11.71	1788.3	6.48	12.19*	1546.9	[6.29]
Unknown CHZI XLIII [m/z 200, 185 (82), 143 (54), 157 (36), 123 (34), 128 (32)...]				12.24	1551.0	0.30
Eudesma-5,7(11)-diene	11.40	1762.3	0.50	12.33*	1558.4	[2.55]
Eremophila-1(10),11-dien-9 β -ol	12.07	1819.9	2.12	12.33*	1558.4	[2.55]
Unknown CHZI XIII [m/z 81, 200 (55), 143 (36), 93 (33),				12.44	1566.4	0.16

91 (32), 185 (31), 129 (27), 128 (21)...						
Unknown CHZI V [m/z 202, 187 (63), 145 (43), 159 (34), 131 (29), 91 (22), 117 (20)]	12.38*	1847.7	[0.73]	12.60	1579.2	1.31
Khusimone				12.72	1588.9	0.41
β -Oplophenone?	15.61	2148.2	0.15	12.92	1604.1	0.16
Unknown MECA V [m/z 179, 161 (66), 119 (44), 95 (38), 105 (35)... 204 (24), 222 (1)]	14.97	2085.4	0.18	12.96	1607.4	0.21
Junenol	13.88	1982.7	0.33	13.00*	1610.9	[2.49]
Unknown CHZI VI [m/z 187, 202 (86), 145 (25), 131 (19), 105 (16), 188 (15)]	12.90	1893.1	1.59	13.00*	1610.9	[2.49]
Selin-6-en-4 α -ol	15.92	2179.5	0.43	13.07	1616.9	0.11
Unknown CHZI XXV [m/z 145, 59 (97), 161 (87), 218 (76), 43 (76), 179 (63)...				13.19	1626.5	0.62
Unknown VEAC II [m/z 43, 161 (92), 204 (54), 147 (46)... 145 (20), 220 (17)]				13.24	1631.1	1.03
τ -Cadinol	15.18	2106.6	0.35	13.31	1636.8	0.76
Unknown CHZI II [m/z 121, 107 (69), 93 (64), 79 (60), 177 (59), 136 (58), 91 (57), 41 (56)... 220 (21)]	15.64	2151.9	1.31	13.40	1644.0	1.17
Unknown CHZI XV [m/z 161, 59 (67), 95 (45), 93 (40), 105 (40), 149 (39), 81 (39), 43 (38), 204 (37)... 220 (5)]	14.94	2082.5	0.38	13.43*	1646.9	[1.74]
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	15.49	2136.9	0.56	13.43*	1646.9	[1.74]
Cyclocopacamphan-12-ol, epimer A	16.58	2246.7	0.79	13.43*	1646.9	[1.74]
Cyclocopacamphan-12-ol, epimer B	16.66	2254.6	0.71	13.52	1654.3	1.42
Zizanone analog				13.59	1659.6	0.39
Zizanol	17.12	2302.0	1.14	13.64	1663.6	1.48
Khusiol	16.34	2221.5	1.15	13.69	1668.2	1.45
epi-Zizanone	15.56	2143.7	0.58	13.74	1672.6	0.22
Zizanal	17.51	2343.5	0.37	13.78	1675.8	0.76
Unknown CHZI XXVI [m/z				13.89	1684.4	1.27

189, 43 (91), 81 (89), 105 (81), 91 (74), 93 (74), 133 (67), 41 (67)... 222 (37)]						
Unknown CHZI I [m/z 189, 159 (82), 133 (44), 91 (29), 105 (29), 205 (25)... 220 (13)]	17.23	2314.1	3.11	14.11	1702.9	3.36
Vetiselinol	17.42	2334.5	1.18	14.24	1714.2	1.74
Khusimol	18.13*	2410.1	[5.84]	14.45	1732.2	5.91
Unknown CHZI XXIII [m/z 189, 187 (29), 159 (23), 43 (20), 133 (16)...]				14.51	1737.4	0.30
10-epi-Acora-3,11-dien-15-al?				14.55*	1741.0	[0.84]
γ-Costol	18.39	2439.0	0.12	14.55*	1741.0	[0.84]
Unknown CHZI XXXVIII [m/z 174, 131 (37), 159 (25), 91 (20), 175 (14)...]	17.88	2383.3	0.25	14.87*	1769.0	[0.60]
13-Hydroxyvalencene?				14.87*	1769.0	[0.60]
(E)-Isovalencenol	18.44	2444.7	0.79	14.98	1778.5	1.22
Isozizanoic acid	22.94	2984.1	2.80	15.14*	1791.9	[2.94]
Unknown CHZI VII [m/z 120, 121 (93), 93 (85), 105 (74), 119 (68), 91 (58), 123 (49)... 220 (8)]	18.70	2473.1	0.26	15.14*	1791.9	[2.94]
Nootkatone	18.13*	2410.1	[5.84]	15.15	1793.4	0.25
(Z)-Isovalencenal	17.47	2339.6	0.61	15.23	1800.3	0.91
β-Vetivone	17.96	2392.2	1.96	15.29*†	1805.5	[2.85]
Zizanoic acid	23.74	3089.6	4.01	15.37*†	1812.4	[3.70]
(E)-Isovalencenal	17.66	2359.2	0.54	15.40	1815.3	0.51
Unknown VEAC XXVIII [m/z 159, 202 (40), 187 (24), 145 (17)... 262 (6)]				15.48	1822.3	0.34
α-Vetivone	18.28	2426.8	2.28	15.53	1827.3	2.07
(E)-Eremophila-1(10),7(11)-dien-12-yl acetate	16.90	2278.6	0.17	15.74	1846.2	0.29
(E)-Isovalencenyl acetate?	17.18	2308.3	0.83	15.83	1854.0	0.07
Isovalencenal isomer I?				16.17	1885.3	0.08
β-Cyclodihydrocostunolide?				16.48	1914.3	0.11
Cembrene?	15.32	2120.0	0.36	16.54	1919.1	0.17
Total reported		75.51%			85.13%	

*: 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

Essential Oil, *Chrysopogon zizanioides* ct. Indonesia

Internal code: 24F11-PTH01

Vetiver - Indonesia - Lot: V30111R

Report prepared for:

Plant Therapy

†: 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