

Date : 2024-09-12

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24H28-NPA03

Customer Identification : Benzoin - Vietnam - NP0369 - NPS00173

Type : Essential Oil

Source : *Styrax benzoin*

Customer : Nature Packaged

Checked and approved by:

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

Notes: This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.

This report is an update from the first version issued on 2024-09-12 to format it for online publication.

GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-004 - Terpenes and volatiles profiling by response factor

Results : See analysis summary (next page)

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

Date : 2024-09-06

PHYSICOCHEMICAL DATA

CONCLUSION

This sample is carried in propylene glycol, a dilution that is expected to make the concrete pourable.

In Siam benzoin (expected from Vietnam), benzyl benzoate should be a major constituent, above the content of benzoic acid.^{1,2} We recommend this observation is taken into account when evaluating this batch.

REFERENCES

- (1) Tisserand, R.; Young, R. *Essential Oil Safety*, 2nd ed.; Churchill Livingstone Elsevier, 2014.
- (2) Strub, D. J.; Strub, M.; Baldovini, N. The Resinoids: Their Chemistry and Uses. In *Natural Flavours, Fragrances, and Perfumes*; Gopi, S., Sukumaran, N. P., Jacob, J., Thomas, S., Eds.; Wiley, 2023; pp 115–132. <https://doi.org/10.1002/9783527824816.ch7>.

ANALYSIS SUMMARY

Identification	mg/g	% m/m	Class
Propylene glycol	409.36	40.94	Synthetic
Benzoic acid	118.28	11.83	Simple phenolic
2-Hydroxyacetophenone?	2.02	0.2	Simple phenolic
Eugenol	0.15	0.01	Phenylpropanoid
Vanillin	3.88	0.39	Simple phenolic
4-Butylguaiacol	0.10	0.01	Phenylbutanoid
<i>cis</i> -Vanillin propylene glycol acetal	1.10	0.11	Phenolic acetal
<i>trans</i> -Vanillin propylene glycol acetal	0.26	0.03	Phenolic acetal
α -Bisabolol	0.30	0.03	Sesquiterpenic alcohol
Unknown	0.22	0.02	Unknown
(<i>E</i>)-Coniferyl alcohol	0.56	0.06	Phenylpropanoid
Benzyl benzoate	2.88	0.29	Phenolic ester
Palmitic acid	0.33	0.03	Aliphatic acid
Unknown	4.92	0.49	Unknown
Unknown	2.01	0.2	Unknown
3-(4-Hydroxy-3-methoxyphenyl)-2-oxopropyl benzoate	7.38	0.74	Phenylpropanoid ester
Consolidated total	553.75	55.38	

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

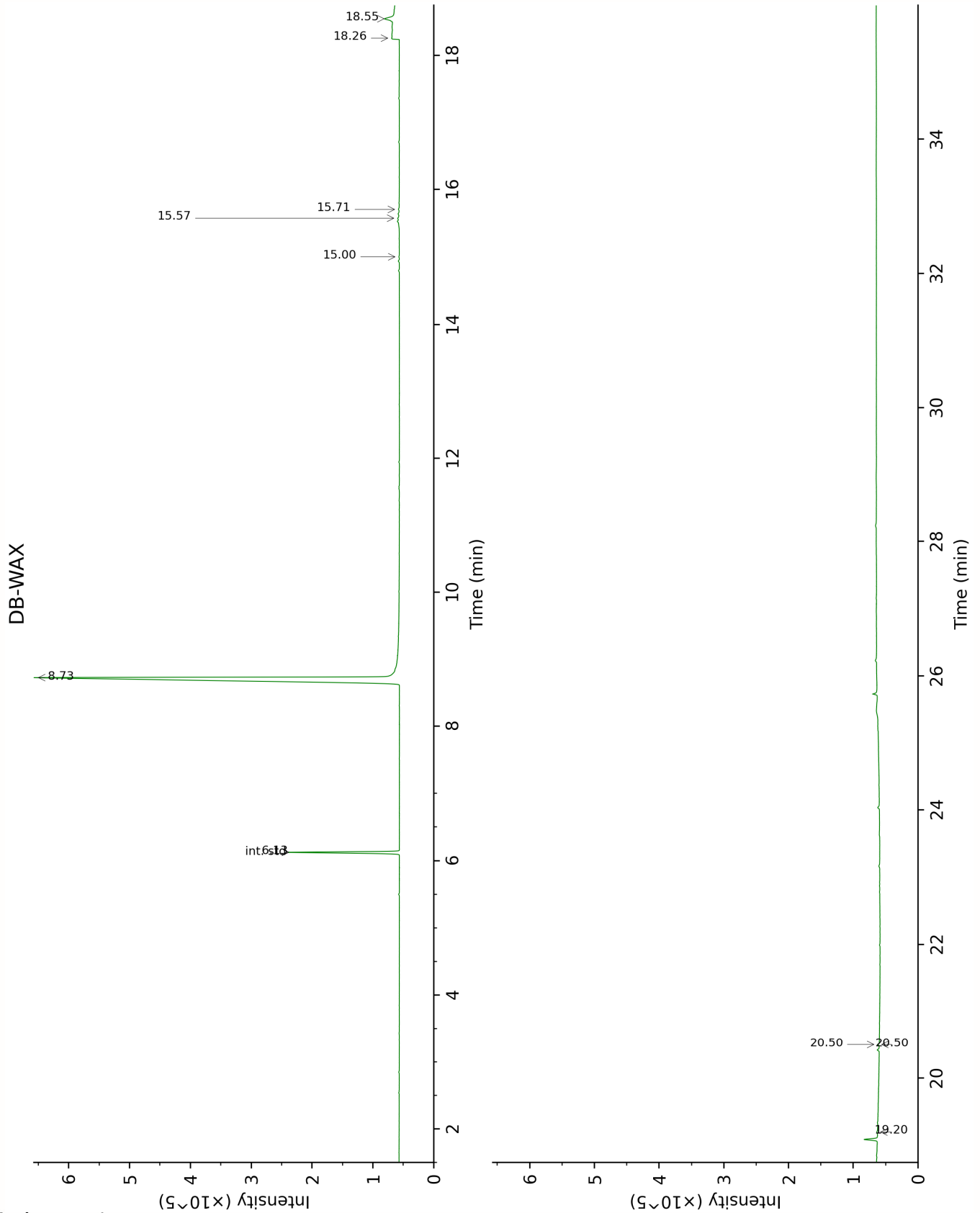
Note: Individual compounds contents were corrected following the method of Cachet et al., 2016 (Flavour and Fragrance Journal guidelines).

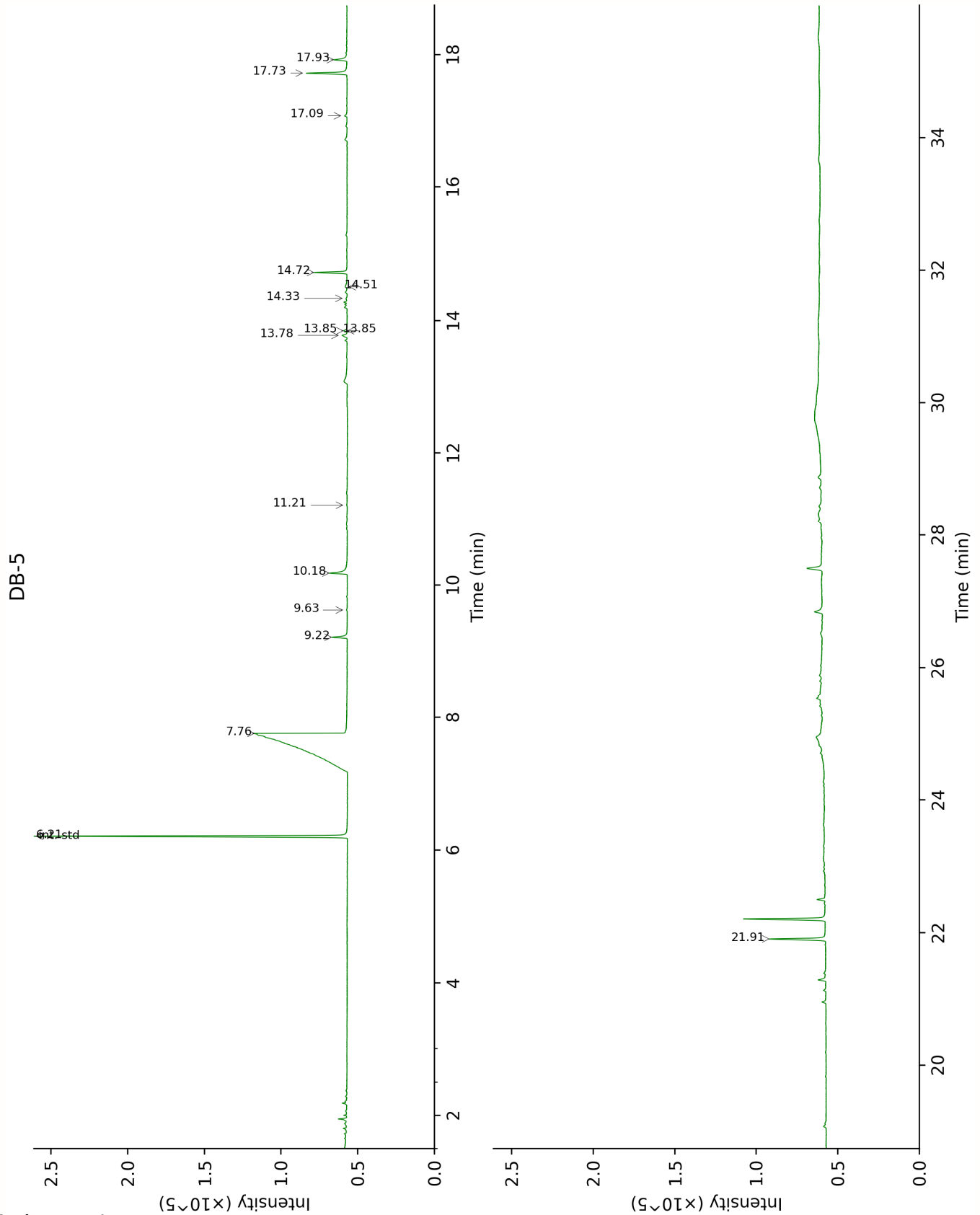
Unknown compounds are expressed in equivalents of internal standard without correction.

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: 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.





FULL ANALYSIS DATA

Propylene glycol	Column DB-WAX			Column DB-5		
	8.73	1548.2	61.75	1.34	778.1	53.81
Benzoic acid	18.26*†	2432.8	[5.08]	7.76	1226.8	25.52
2-Hydroxyacetophenone?				9.22	1325.3	0.46
Eugenol	15.00	2092.7	0.04	9.63	1354.1	0.04
Vanillin	18.55*†	2464.9	[9.06]	10.18	1393.2	0.75
4-Butylguaiacol	15.58	2149.5	0.19	11.22	1469.5	0.02
cis-Vanillin propylene glycol acetal	20.50*†	2694.1	[1.88]	13.78	1672.2	0.22
trans-Vanillin propylene glycol acetal	20.50*†	2694.1	[1.88]	13.85*	1677.8	[0.14]
α-Bisabolol	15.70	2162.5	0.10	13.85*	1677.8	[0.14]
Unknown MISC CXXXVII [m/z 137, 122 (30), 105 (22), 196 (19), 77 (17)...]				14.33	1718.7	0.05
(E)-Coniferyl alcohol				14.51	1733.8	0.12
Benzyl benzoate	19.20*†	2539.6	[1.39]	14.72	1752.3	0.79
Palmitic acid				17.08	1967.1	0.09
Unknown STBE IV [m/z 131, 103 (46), 163 (34), 91 (33), 238 (31)...]				17.73	2029.2	1.14
Unknown STBE V [m/z 131, 103 (48), 91 (39), 119 (37), 163 (36)...]				17.93	2049.2	0.47
3-(4-Hydroxy-3-methoxyphenyl)-2-oxopropyl benzoate				21.91	2479.2	1.51
Total reported		96.21%			91.48%	

*: 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