

Supplemental Material

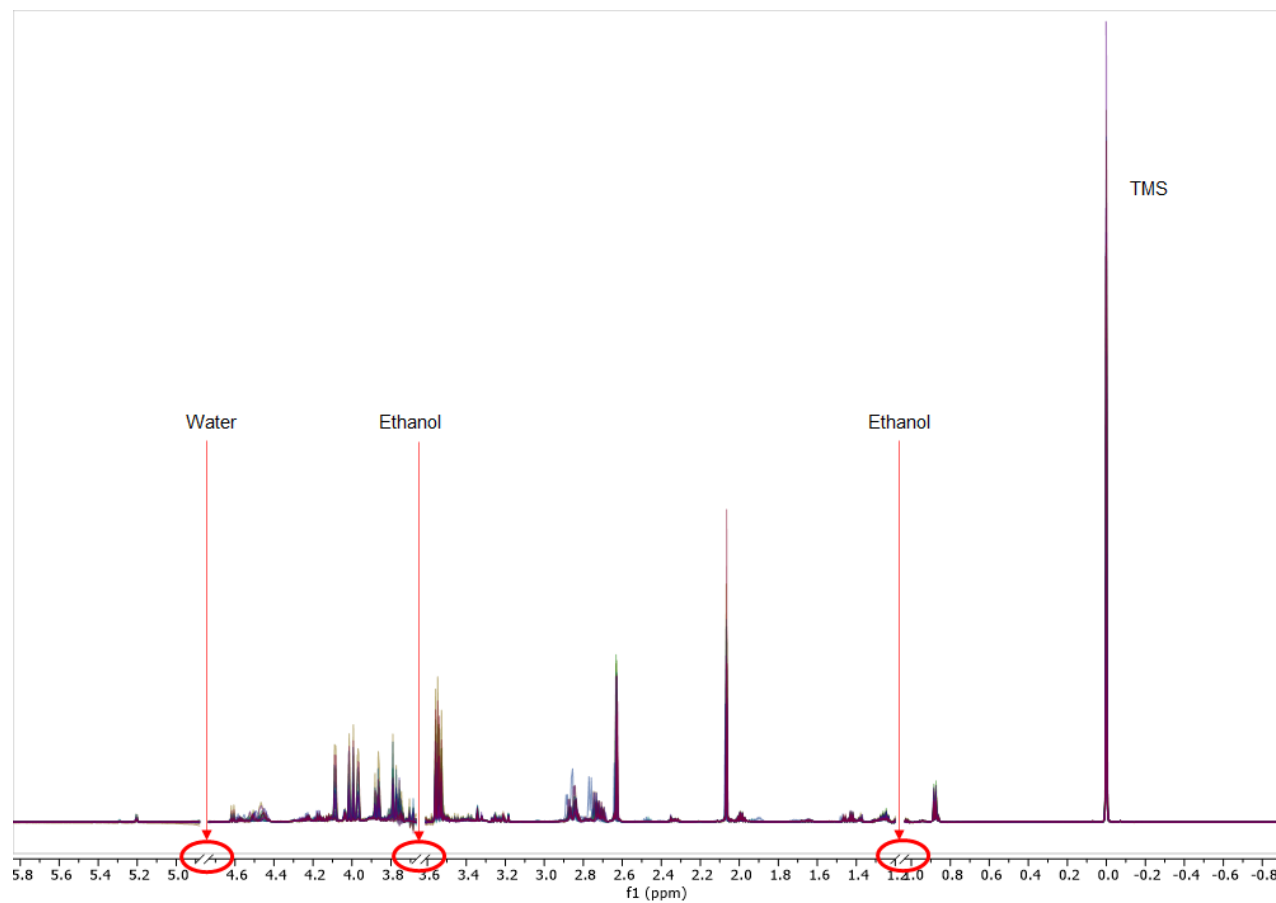


FIGURE S1. Nuclear Magnetic Resonance (NMR) spectral overlay for the 23 experimental wines analysed in Year 2.

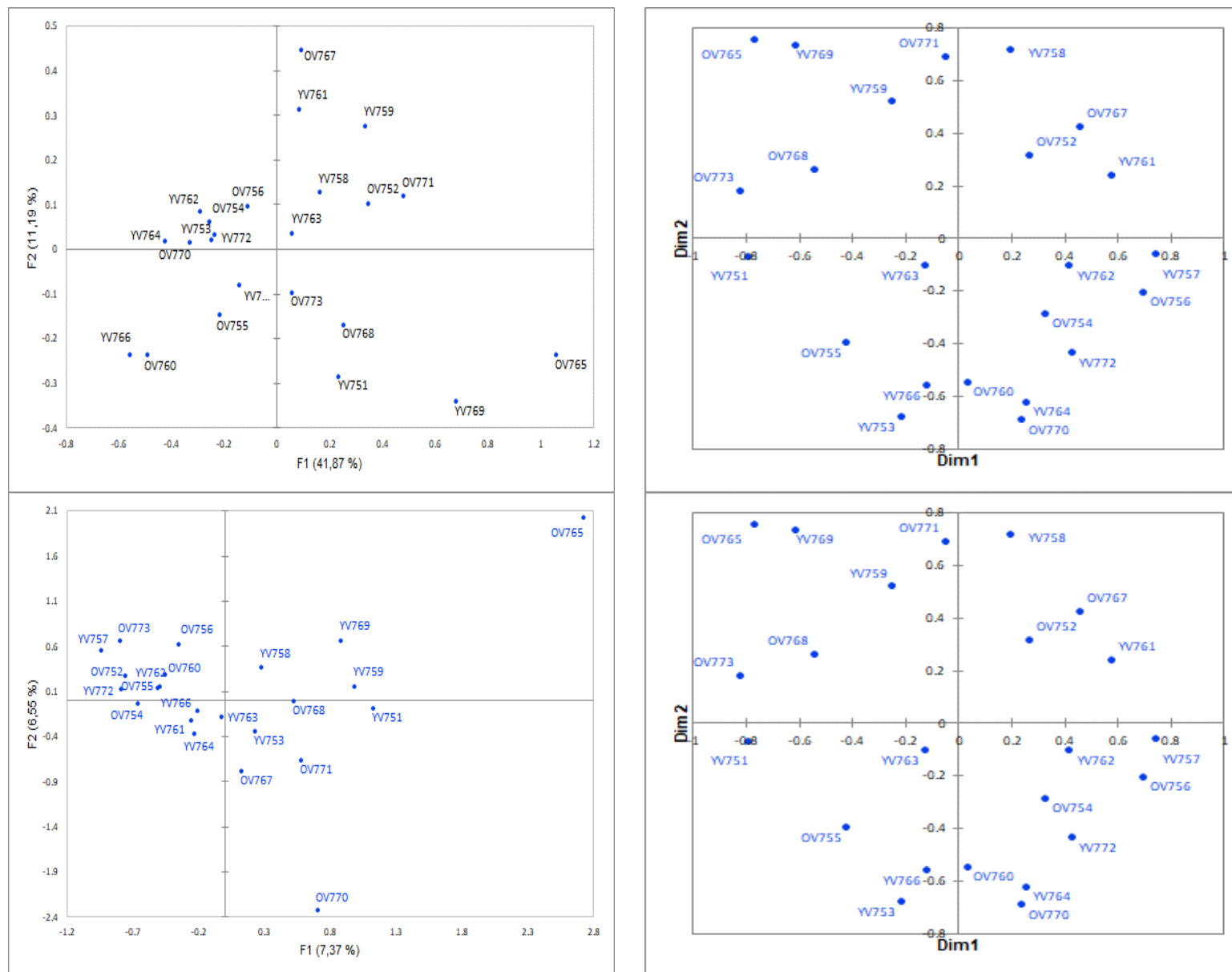


FIGURE S2. Sensory biplot projections for verbal (left) and non-verbal (right) aspects for Year 1 (above) and Year 2 (below).

SUPPLEMENTARY DATA

Mafata, M., Brand, J., & Buica, A. (2022). Data fusion using Multiple Factor Analysis coupled with non-linear pattern recognition (fuzzy k-means): application to Chenin blanc. *OENO One*, 56(3).
<https://doi.org/10.20870/oeno-one.2022.56.3.5374>

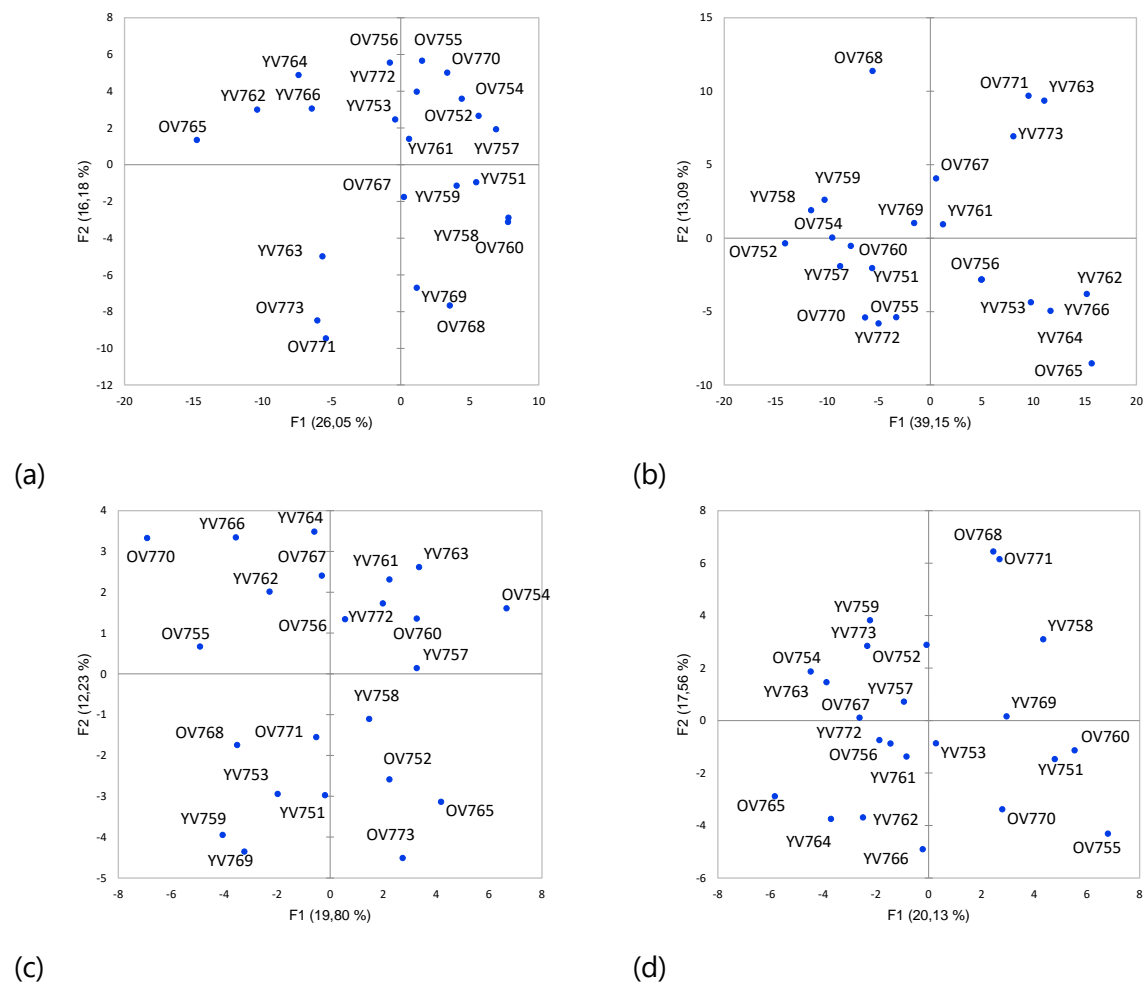
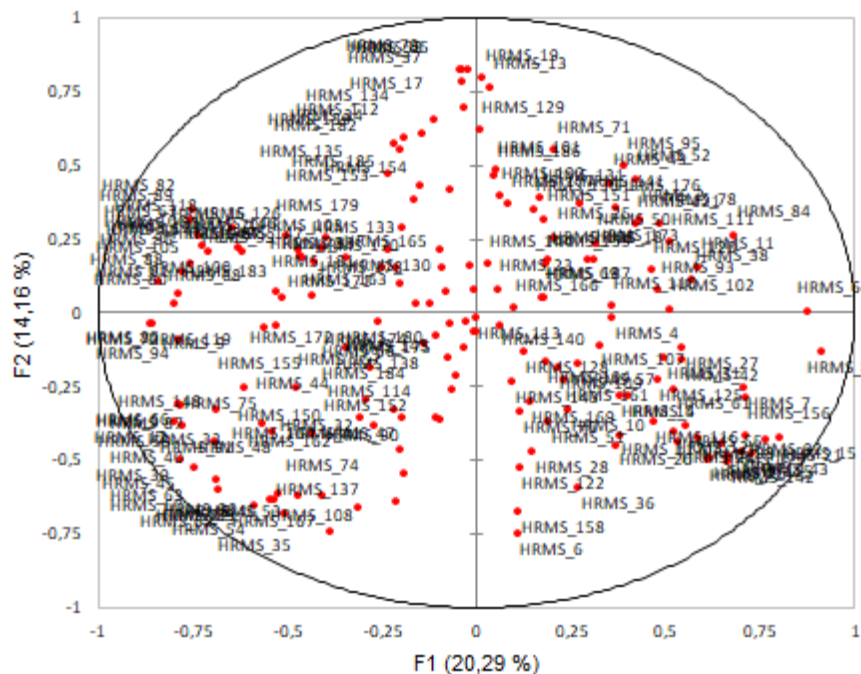
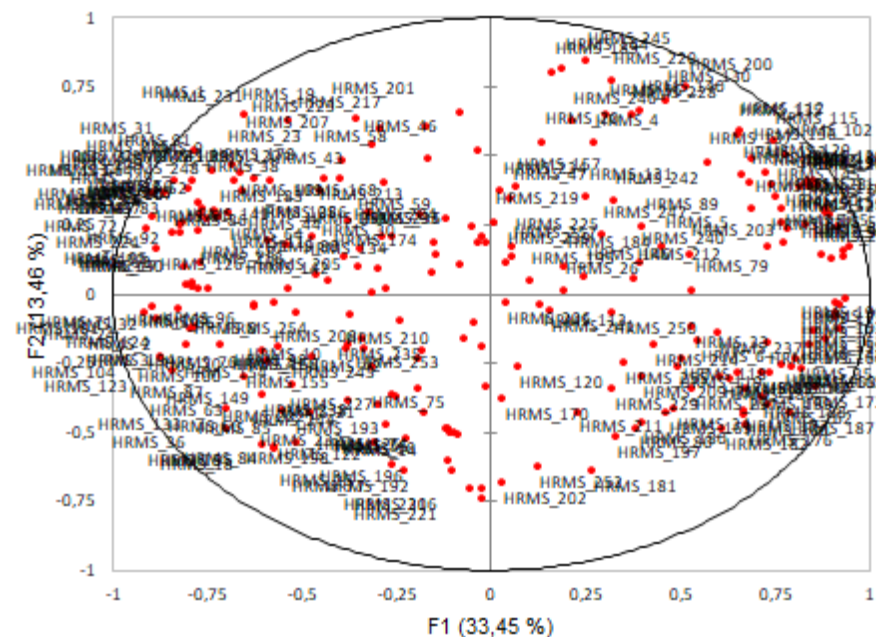


FIGURE S3. Block PCA analysis on HRMS data acquisition in positive mode for Year 1 (a) and Year 2 (b), and negative mode for Year 1 (c) and Year 2 (d).



(a)

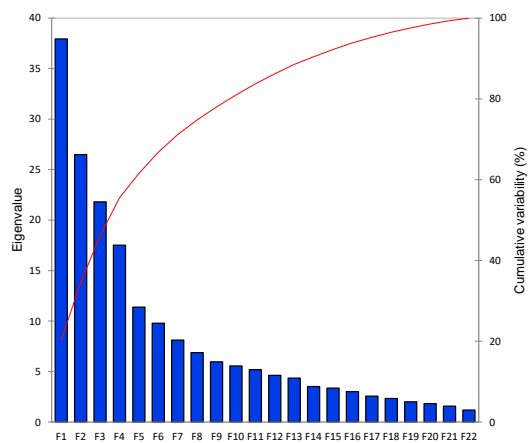


(b)

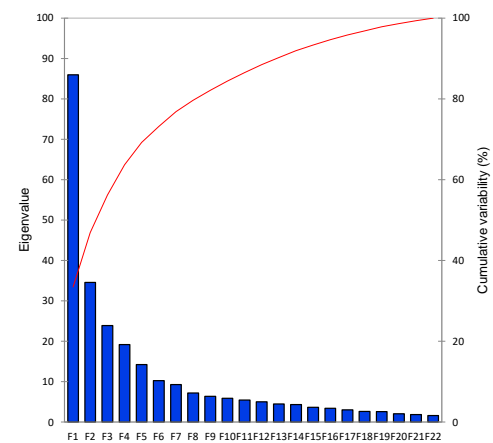
FIGURE S4. PCA loadings of HRMS in combined (Pos. and Neg.) acquisition modes for (a) Year 1 and (b) Year 2.

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(a)

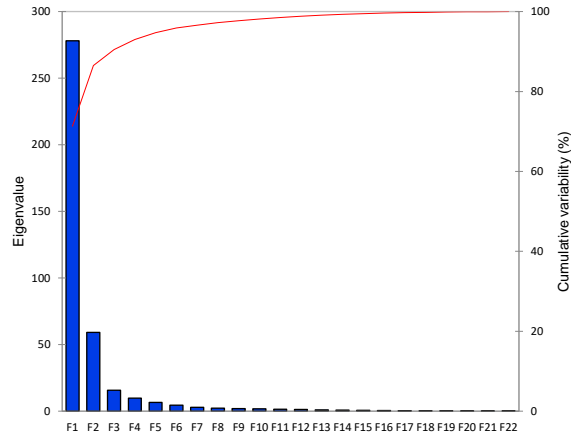


(b)

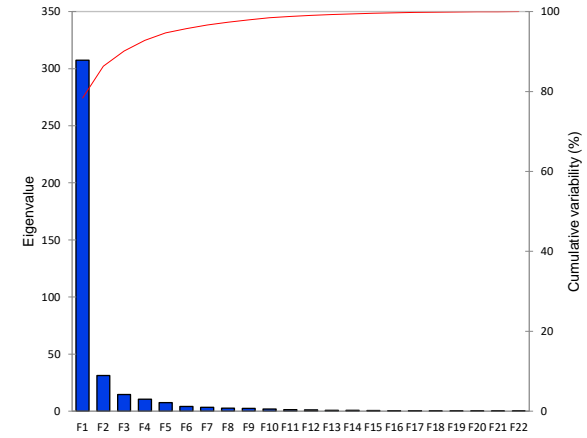
FIGURE S5. Scree plot for PCA of the combined HRMS (Positive and negative) of (a) Year 1 and (b) Year 2.

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(a)



(b)

FIGURE S6. Scree plot of the PCA of the complete NMR data for (a) Year 1 and (b) Year 2.

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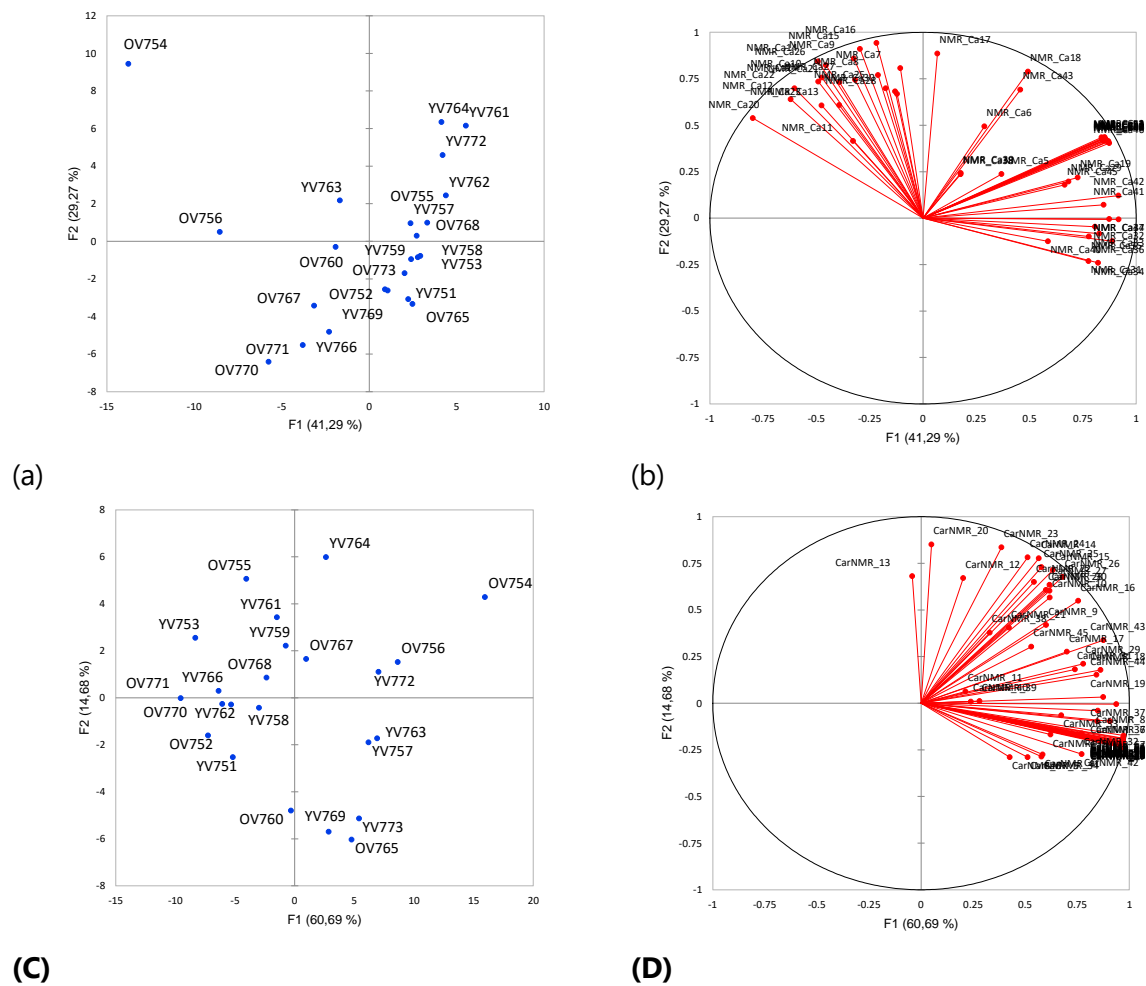
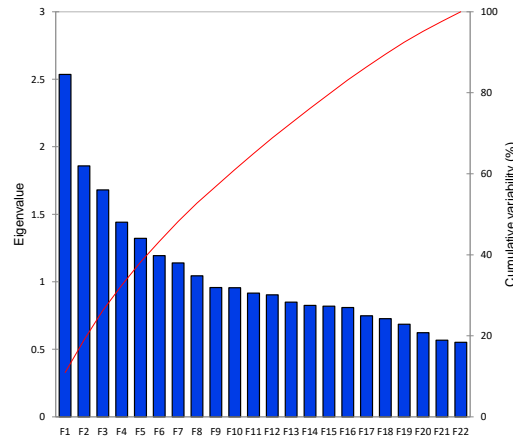


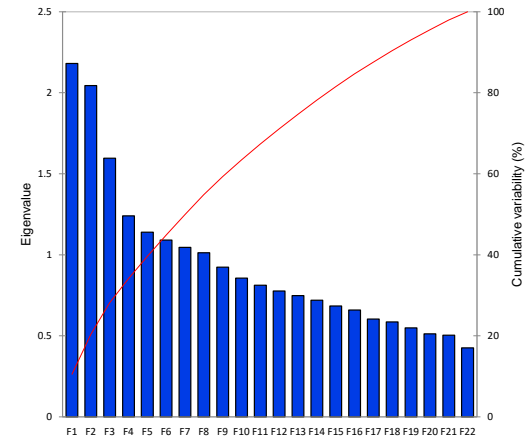
FIGURE S7. PCA of Carbohydrate region of the NMR for Year 1 (a) scores and (b) loading, and Year 2 (c) scores and (d) loadings.

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<https://doi.org/10.20870/oenone.2022.56.3.5374>



(a)



(b)

FIGURE S8. Scree plot for the MFA data fusion model of (a) Year 1 and (b) Year 2.

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TABLE S1. Pairwise RV coefficients between the three NMR regions (Aryl, Aromatic and carbohydrate) for Year 1 and Year 2 data exploration.

Year 1					Year 2				
	Alkyl	Carbs	Aromatics	MFA		Alkyl	Carbs	Aromatics	MFA
Alkyl	1	0.716	0.554	0.852	Alkyl	1.000	0.813	0.807	0.924
Carbs	0.716	1	0.769	0.943	Carbs	0.813	1.000	0.914	0.960
Aromatics	0.554	0.769	1	0.864	Aromatics	0.807	0.914	1.000	0.956
MFA	0.852	0.943	0.864	1	MFA	0.924	0.960	0.956	1.000

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TABLE S2. Fuzzy k-means clustering at F_k set at 1.001 and the number samples at 22 for Year 1 and 21 for Year 2.

Year 1					Year 2				
Number of clusters	Criterion	Between-classes	Within-class variance	Wilks' Lambda test	Number of clusters	Criterion	Between-classes	Within-class variance	Wilks' Lambda test
1	1.000	0.000	487.658	1.000	1	1.000	0.000	399.889	1.000
2	0.996	218.181	269.478	0.553	2	0.995	177.728	222.160	0.556
3	0.988	284.711	202.947	0.416	3	0.986	234.489	165.399	0.414
4	0.976	316.788	170.871	0.350	4	0.975	260.357	139.532	0.349
5	0.961	336.322	151.337	0.310	5	0.957	274.137	125.751	0.314
6	0.945	352.778	134.880	0.277	6	0.943	289.119	110.769	0.277
7	0.932	369.635	118.023	0.242	7	0.925	300.846	99.043	0.248
8	0.922	385.240	102.418	0.210	8	0.916	315.501	84.387	0.211
9	0.923	402.286	85.372	0.175	9	0.924	329.859	70.030	0.175
10	0.944	416.330	71.329	0.146	10	0.961	340.511	59.378	0.148
11	0.998	423.323	64.335	0.132	11	0.998	362.560	37.329	0.093
12	0.998	446.013	41.646	0.085	12	0.998	365.707	34.181	0.085

Table S3. Variance decomposition for the optimal classification for Year 1 and Year 2 clustering using parametric (Agglomerative hierarchical clustering - AHC) and non-parametric (Fuzzy k-means) methods.

	Year 1			Year 2		
		Absolute	Percent		Absolute	Percent
AHC with all samples	Within-class	22.308	90.95 %	Within-class	19.96	88.57 %
	Between-classes	2.219	9.05 %	Between-classes	2.575	11.43 %
	Total	24.528	100.00 %	Total	22.535	100.00 %
		Absolute	Percent		Absolute	Percent
AHC without outliers	Within-class	22.308	96.07 %	Within-class	19.051	95.28 %
	Between-classes	0.913	3.93 %	Between-classes	0.944	4.72 %
	Total	23.222	100.00 %	Total	19.994	100.00 %
		Absolute	Percent		Absolute	Percent
Fuzzy k-means clustering	Within-class	1.835	15.93 %	Within-class	10.084	87.30 %
	Between-classes	9.688	84.07 %	Between-classes	1.466	12.70 %
	Total	11.524	100.00 %	Total	11.55	100.00 %