

SUPPLEMENTARY MATERIAL

Study of the minor fraction of virgin olive oil by a multi-class GC-MS approach: Comprehensive quantitative characterization and varietal discrimination potential

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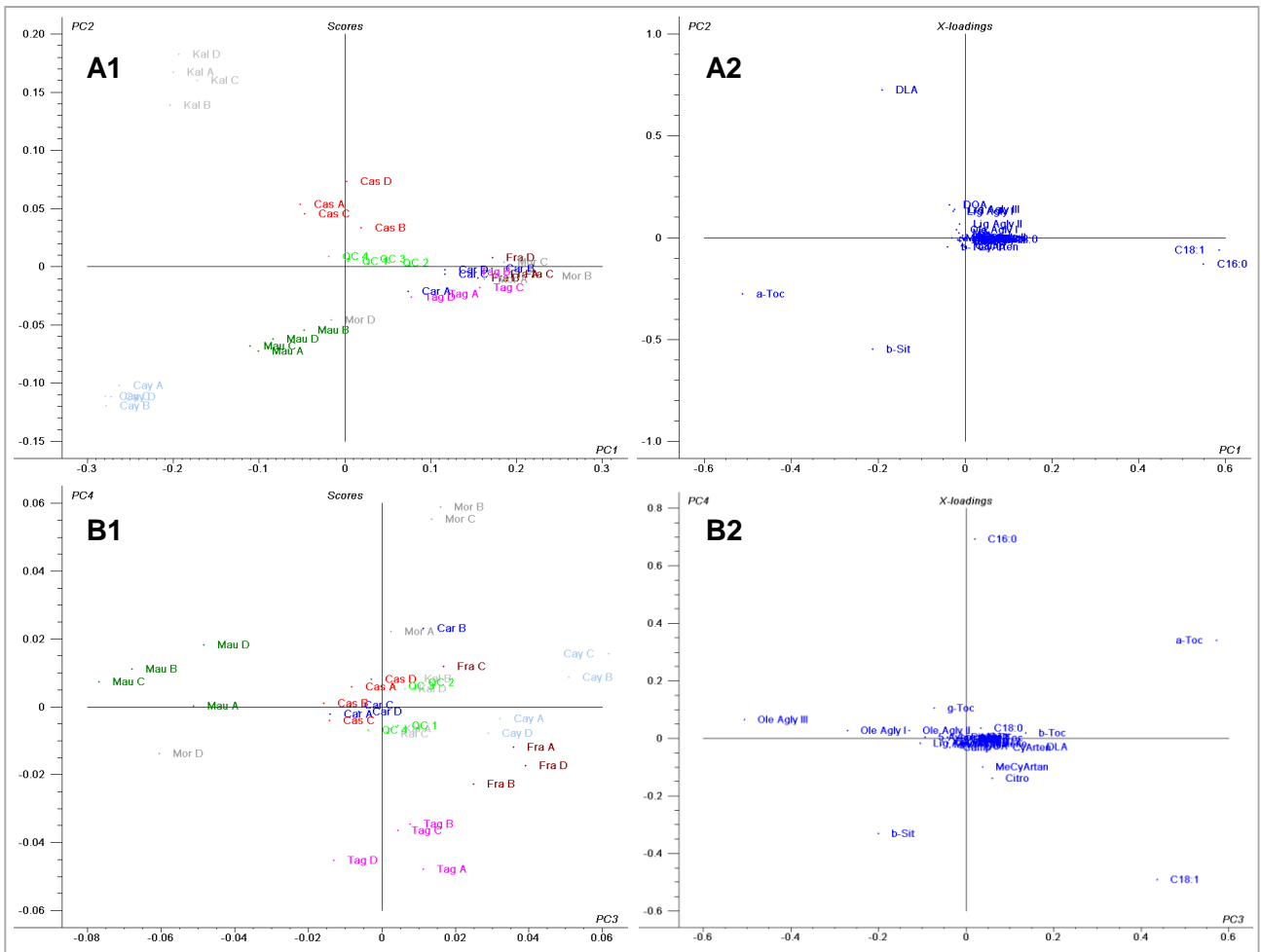
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Table 1 SM. Identified compounds in GC-MS.

<i>Rt</i> (min)	<i>Compound</i>	<i>m/z characteristic signals</i>	<i>Assigned formula to the m/z signals in bold letters</i>
6.9	Van	194/209/ 224 /45	M-H+TMS
7.8	TY	179/267/ 282 /180	M-2H+2TMS
12.8	HTY	267/ 370 /73/193	M-3H+3TMS
14.1	AcHTY	280/73/193/ 340	M-2H+2TMS
14.7	EA I	153/299/196/ 314	M-H+TMS
15.3	Qui	346 /256/73/419	M-5H+5TMS-2TMSO-CO
16.3	EA II	73/178/165/ 314	M-H+TMS
17.2	<i>p</i> -Cou	294/73/ 308 /250	M-2H+2TMS
19.3	C16:1	312/129/117/ 326	M-H+TMS
19.9	C16:0	117/314/129/ 328	M-H+TMS
20.8	Fer	338 /324/294/73	M-2H+2TMS
23.5	C18:2	338/73/129/ 352	M-H+TMS
23.8	C18:1	354 /117/129/340	M-H+TMS
24.3	C18:0	342/117/129/ 356	M-H+TMS
29.9	DLA	192/177/73/ 361	M-H+TMS-CH ₃
33.1	DOA	280/73/193/ 464	M-2H+2TMS
34.9	LigAgly I	192 /73/280/ 177	(Olmo-García et al., 2018)
36.1	LigAgly II	192 /73/ 177 /297	(Olmo-García et al., 2018)
36.6	δ -Toc	475 /209/73/249	M-H+TMS
37.0	LigAgly III	193/73/ 417 /177	M-2H+2TMS-TMSO
37.6	OleAgly I	280/73/193/ 522	M-2H+2TMS
37.9	β -Toc	489 /223/73/41	M-H+TMS
38.1	γ -Toc	489 /223/73/43	M-H+TMS
38.7	OleAgly II	280/73/45/ 505	M-3H+3TMS-TMSO
39.5	OleAgly III	280/73/193/ 594	M-3H+3TMS
40.3	α -Toc	503 /238/73/43	M-H+TMS
40.4	Api	472/45/399/ 486	M-3H+3TMS
41.8	Cam	503/ 472 /73/383	M-H+TMS
42.2	Sti	395/ 485 /83/256	M-H+TMS
42.6	Lut	560/45/472/ 574	M-4H+4TMS
43.1	β -Sit	397/358/ 486 /381	M-H+TMS
43.2	Pin	502 /223/235/488	M-2H+2TMS
43.3	Δ^5 -Ave	386/297/282/ 484	M-H+TMS
43.7	AcPin	276/246/546/ 560	M-2H+2TMS
44.1	CyArten	393/366/ 408 /69	M-H+TMS-TMSOH
44.9	MeCyArtan	408/380/422/ 512	M-H+TMS
45.4	ER	497 /216/73/203	M-2H+2TMS-TMSO
45.4	Cit	358/400/268/ 394	M-H+TMS-TMSOH-CH ₂
45.9	UV	497 /73/216/203	M-2H+2TMS-TMSO
46.3	OA	203/ 483 /73/320	M-2H+2TMS-TMSO-CO
46.6	BA	189/73/203/ 483	M-2H+2TMS-TMSO-CO
47.0	UA	320/203/73/ 483	M-2H+2TMS-TMSO-CO
48.6	MA	203/73/ 571 /320	M-3H+3TMS-TMSO-CO

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Fig. 1 SM. Scores plot (1) and loadings plot (2) for PC1 vs. PC2 (A) and PC3 vs. PC4 (B) charts of the PCA model.



Abbreviations: Car (Carolea), Cas (Casaliva), Cay (Cayon), Fra (Frantoio), Kal (Kalamon), Mau (Maurino), Mor (Moraiolo), QC (Quality Control Samples) and Tag (Taggiasca).