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Supplementary Material

Headspace gas chromatography coupled to mass spectrometry and ion mobility spectrometry: Classification of virgin olive oils as a study case

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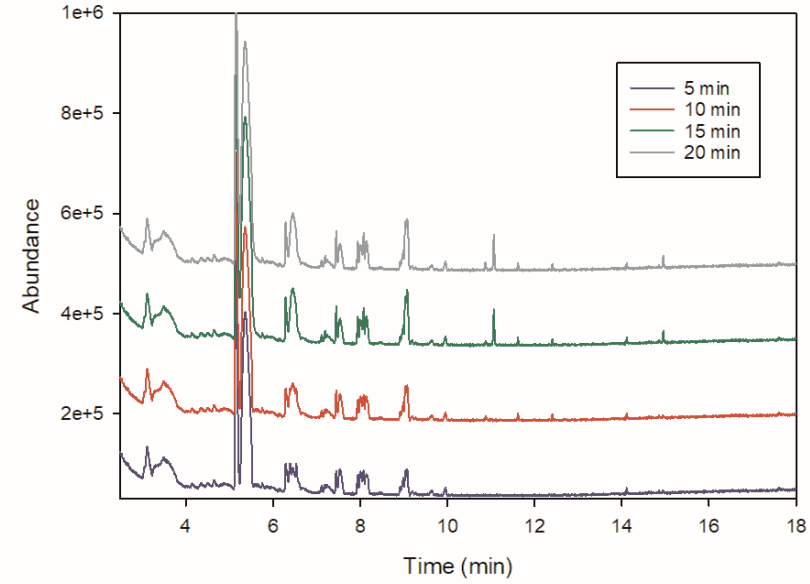
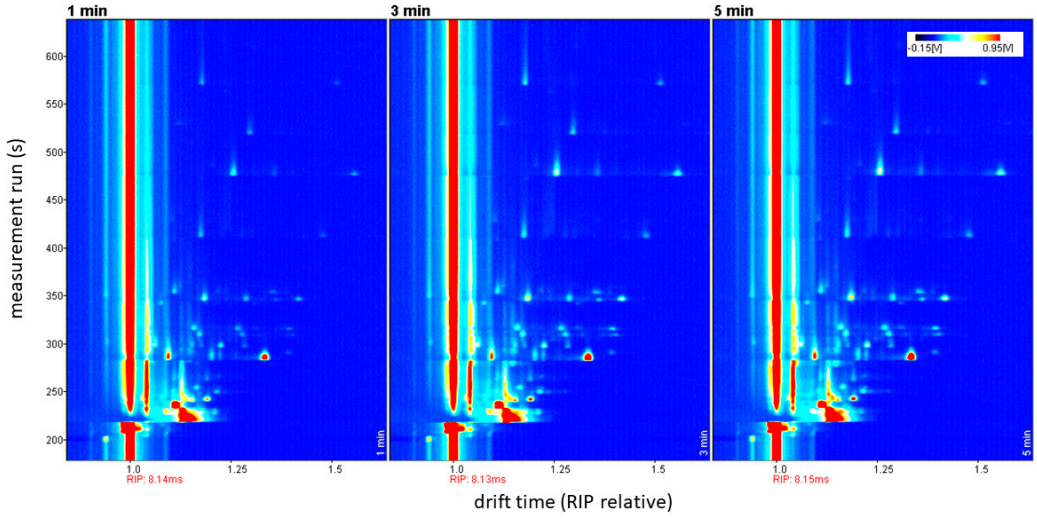
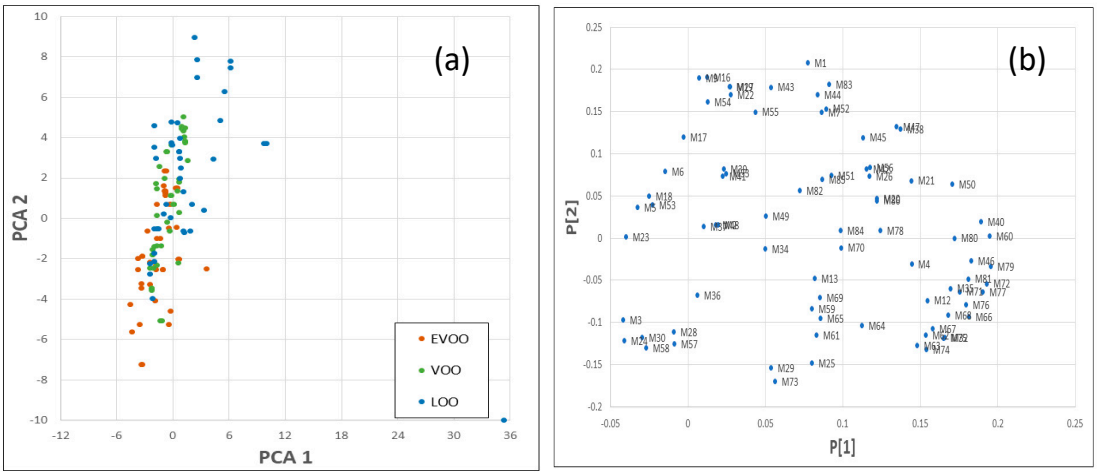


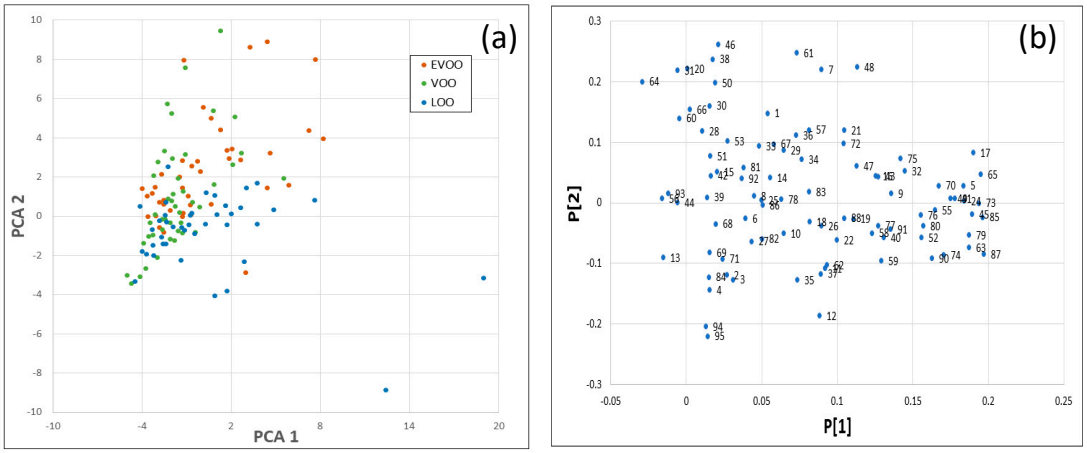
Supplemental Figure S1. HS-GC-MS chromatogram obtained for 5, 10, 15 y 20 minutes of incubation time



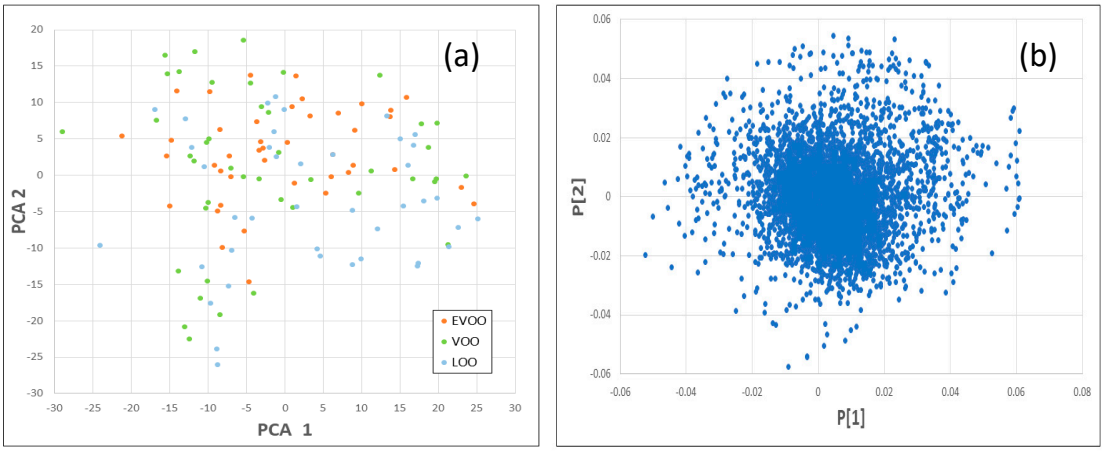
Supplemental Figure S2. HS-GC-IMS spectra obtained for 1, 3 y 5 minutes of incubation time



Supplemental Figure S3. PCA scores and loading plot using the HS-GC-IMS markers



Supplemental Figure S4. PCA scores and loading plot using the peak integration of the HS-GC-MS method



Supplemental Figure S5. PCA scores and loading plot using the TIC of the HS-GC-MS method.

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Supplemental Table S1. Chemical information of the VOCs monitored

		Molecular formula	Molecular weight	*m/z* theoretical ions
Alcohols	1-octanol	$C_8H_{18}O$	130.22	56, 41, 43, 55, 70, 69, 84, 83, 29, 31
	1-pentanol	C5H12O	88.14	42, 56, 41, 70, 31, 29, 57, 43
	1-hexanol	C6H14O	102.17	56, 43, 41, 55, 31, 27, 29, 69
	2-methyl-1-butanol	C5H12O	88.14	57, 41, 56, 70, 29
	3-methyl-1- butanol	C5H12O	88.14	55, 42, 43, 41, 70. 31, 29, 27, 39, 57
	trans-2-hexen-1-ol	C6H12O	100.15	51, 41, 82, 44, 67. 27, 29, 71
	cis-2-penten-1-ol	C5H10O	83.13	57, 41, 39, 44, 29, 58, 67, 55
	2-octanol	C8H18O	130.22	45, 55
	1-octen-3-ol	C8H16O	128.12	57, 43, 72, 85, 41, 29, 99
Ketones	2-butanone	C4H8O	72.1	43, 72, 29, 57
	2-pentanone	C5H10O	86.13	43, 86, 41, 58, 71, 27
	1-penten-3-one	C5H8O	84.11	55, 27, 84
	2-hexanone	C6H12O	100.15	43, 58, 41, 100, 85, 71, 39
	2-heptanone	C7H14O	114.18	43, 58, 71, 27, 29
	1-octen-3-one	C8H14O	126.19	55, 70, 27. 43, 41, 39
	2-octanone	C8H16O	128.21	43, 58, 41, 71, 85
	2-nonanone	C9H18O	142.23	43, 58, 41, 71, 27, 29, 57, 142
	4-methyl-penan-2-one	C6H12O	100.15	43, 58, 41, 85, 100, 39, 29
	6-methyl-5-hepten-2-one	C8H14O	126.19	43, 41, 55, 69, 108, 111, 126, 58
Aldehydes	hexanal	C6H12O	100.15	44, 56, 41, 43, 57, 29, 43, 72, 82
	trans-2-hexen-1-al	C6H10O	98.14	41, 42, 39, 55, 57, 69, 83, 98
	trans-2-pentenal	C5H8O	84.12	55, 84, 83,41, 39, 29, 27, 53, 69
	decanal	C10H20O	156.26	43, 41, 55, 57 29, 70, 68, 82, 112, 95
	trans-2-decenal	C10 H18 O	154.24	43, 41, 29, 55, 70, 83, 57, 39, 27, 98, 110, 136

	octanal	C8H16O	128.21	43, 56, 44, 41, 84, 57, 55, 29, 27, 69, 82
	trans-2-heptenal	C7H12O	112.17	41, 27, 28, 39, 55, 57, 43, 83, 70
	heptanal	C7H14O	114.18	70, 41, 44,43, 55, 57, 29, 39, 27, 81, 86, 96
	nonanal	C9H18O	142.24	57, 41, 43, 56, 29, 27, 55, 98, 70, 69, 82
	trans-2-octenal	C8H14O	126.2	41, 55, 70, 83, 29, 57, 39, 67
Esters	ethyl acetate	C4H8O2	88.11	43, 61, 45, 88, 29, 70
	ethyl butyrate	C6H12O2	116.16	71, 43, 88, 29, 60, 73, 41, 45, 101
	ethyl isovalerate	C7H14O2	130.18	88, 57, 29, 85, 60, 41 70
	3-hexenyl acetate	C8H14O2	142.2	43, 41, 53, 55, 69, 67
	propyl butyrate	C7H14O2	130.18	43, 71, 27, 89, 41, 60, 39, 29
	hexyl acetate	C8H16O2	144.21	43, 56, 55, 61, 84, 69, 42, 41, 73
Monoterpenes	limonene	C10H16	136.23	68, 93, 67, 107, 136, 121, 53, 39
Other compounds	n-octane	C8H18	114.23	43, 41, 57, 29, 71, 85
	diethyl phtalate	C12H14O4	222.24	149, 177