

Supplementary Information

The Infestation of Olive Fruits by *Bactrocera oleae* (Rossi) Modifies the Expression of Key Genes in the Biosynthesis of Volatile and Phenolic Compounds and Alters the Composition of Virgin Olive Oil

Andrés Notario, Rosario Sánchez, Pilar Luaces, Carlos Sanz and Ana G. Pérez *

Table S1: Groups of volatile compound (according to their biochemical origin) analyzed in the oils.

	Manzanilla		Picual		Hojiblanca	
Compounds (ng/g oil)	Control	Infested	Control	Infested	Control	Infested
Σ aldehydes C6/LnA	10255,8a	11960,4b	15339,5a	22678,6b	16990,2a	22996,7b
Σ alcohols C6/LnA	1075,1a	1167,5a	2420,6a	4879,7b	1507,1a	5423,4b
Σ C6/LnA	11423,3a	13035,5b	17760,1a	27558,4b	18497,4a	28420,1b
Σ aldehydes C6/LA	1515,8a	1547,1a	1734,9a	2506,2b	3495,9a	3440,0a
Σ alcohols C6/LA	271,4a	282,5a	463,0a	698,8b	341,2a	1129,2b
Σ C6/LA	1787,3a	1829,6a	2197,9a	3205,0b	3837,1a	4569,2b
Σ carbonyls C5/LnA	614,6b	418,2a	878,9b	320,1a	687,0b	409,2a
Σ alcohols C5/LnA	2104,5a	2676,5b	868,7a	1036,2b	796,7b	747,0a
Σ DP	5835,1a	5544,7a	6146,9a	5846,7a	9846,9a	9461,8a
Σ C5/LnA	8544,3a	8639,5a	7894,6a	7203,0a	11330,8a	10618,1a
Σ carbonyls C5/LA	397,4a	527,3b	236,8a	529,2b	278,2a	658,6b
Σ alcohols C5/LA	66,7a	49,0a	103,1a	129,8a	85,0a	132,4b
Σ C5/LA	464,1a	576,4b	339,9a	659,1b	363,3a	791,0b
Σ esters LOX	324,0a	547,9b	215,1a	419,9b	369,7a	410,9b
Σ esters no LOX	1130,0b	600,9a	1028,6a	1490,7b	1108,2b	1002,7a
Σ esters	1454,1b	1148,8a	1243,7a	1910,7b	1477,9a	1413,6a
Σ aldehydes AA	53,2a	108,5b	14,0a	22,65b	45,6a	46,8a
Σ alcohols AA	3,5a	4,3a	9,1a	16,2b	3,8b	2,6a
Σ volatiles AA	56,8a	112,8b	23,1a	38,8b	49,4a	49,4a

Σ terpenes	11753,4b	10864,3a	9096,9a	9054,9a	751,7a	931,2b
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(*) mean contents from three different analyses

(**) different letters within the same olive cultivar indicate statistically significant differences ($p \leq 0.05$)

Table S2

Compounds (ng/g oil)	Picual C			Picual I			Manzanilla C			Manzanilla I			Hojiblanca C			Hojiblanca I		
Ethyl acetate	251.3	±	6.3	568.1	±	14.9	448.4	±	10.1	721.1	±	56.4	502.6	±	14.0	728.9	±	0.3
Ethanol	504.4	±	3.3	912.6	±	32.2	231.4	±	20.9	341.9	±	9.8	767.0	±	54.9	1280.5	±	20.4
E3-hexenal	844.6	±	371.5	1729.6	±	57.5	613.4	±	40.6	283.6	±	15.4	627.3	±	21.0	461.1	±	0.1
Z3-hexenal	9229.6	±	202.8	5277.9	±	94.9	6963.9	±	66.0	3119.0	±	238.8	8946.3	±	538.6	3137.5	±	42.7
Z2-hexenal	776.0	±	24.2	478.0	±	30.6	676.1	±	50.3	332.2	±	13.5	945.3	±	56.3	437.1	±	4.3
E2-hexenal	4489.3	±	95.7	15193.1	±	247.5	3707.0	±	317.1	6521.0	±	214.0	6471.3	±	223.6	18961.0	±	190.9
E3-hexenol	20.6	±	3.5	103.9	±	1.3	10.4	±	0.4	24.4	±	1.0	26.0	±	0.4	31.9	±	1.2
Z3-hexenol	2153.9	±	2.4	3684.6	±	58.0	854.2	±	44.4	875.0	±	7.7	1234.3	±	19.7	3782.3	±	50.5
E2-hexenol	246.1	±	16.3	1091.3	±	42.9	210.6	±	40.2	268.2	±	0.8	246.8	±	4.2	1609.2	±	22.5
hexanal	1734.9	±	60.3	2506.2	±	20.6	1515.9	±	27.2	1547.1	±	58.4	3495.9	±	29.8	3440.1	±	46.3
hexanol	463.0	±	10.4	698.8	±	9.4	271.5	±	36.4	282.5	±	12.2	341.3	±	5.3	1129.2	±	11.1
1-penten-3-one	682.6	±	16.3	198.7	±	5.9	478.5	±	18.1	311.6	±	0.9	506.8	±	25.6	243.1	±	8.6
Z2-pentenal	80.8	±	3.5	23.3	±	0.7	62.7	±	3.7	41.1	±	0.0	69.1	±	3.8	21.0	±	0.5
E2-pentenal	115.6	±	6.4	98.1	±	5.9	73.5	±	8.0	65.5	±	3.9	111.2	±	2.3	145.1	±	5.0
1-penten-3-ol	181.8	±	13.7	126.1	±	6.5	135.0	±	9.8	120.6	±	5.2	158.1	±	6.5	137.1	±	7.5
Z2-pentenol	485.2	±	3.3	576.4	±	10.6	392.5	±	10.0	595.4	±	17.1	336.4	±	7.6	320.1	±	6.2
E2-pentenol	201.7	±	2.3	333.8	±	8.0	1577.0	±	43.9	1960.6	±	37.5	302.3	±	4.2	289.9	±	6.8
DP-1	278.6	±	8.3	252.3	±	6.1	240.5	±	12.7	248.3	±	12.5	501.9	±	34.8	466.2	±	16.1
DP-2	221.0	±	4.8	210.2	±	4.9	200.6	±	8.3	213.9	±	9.6	387.0	±	39.9	364.8	±	6.9
DP-3	1092.5	±	17.8	1105.8	±	0.3	1049.3	±	25.4	1136.7	±	56.3	2069.2	±	44.6	2070.9	±	41.7
DP-4	1985.3	±	40.1	1489.6	±	33.9	1687.7	±	111.2	1501.6	±	141.1	2525.3	±	135.3	2249.6	±	41.7
DP-5	317.0	±	22.0	339.5	±	3.0	365.1	±	9.0	403.0	±	14.1	510.2	±	17.1	568.9	±	19.2
DP-6	1290.8	±	40.5	1265.5	±	64.6	1114.2	±	107.6	1525.4	±	517.1	1740.3	±	245.6	2154.3	±	82.6
DP-7	961.7	±	371.0	1183.9	±	91.0	1177.7	±	320.0	515.9	±	515.9	2113.1	±	350.6	1587.1	±	506.9
2+3-pentanone	170.1	±	19.5	476.7	±	39.7	324.8	±	24.6	444.5	±	30.2	245.8	±	30.6	634.4	±	50.5
pentanal	66.7	±	3.6	52.5	±	2.7	72.6	±	5.0	82.8	±	0.8	32.5	±	10.6	24.2	±	0.5
pentanol	103.1	±	24.7	129.9	±	23.9	66.7	±	4.8	49.1	±	37.6	85.1	±	3.8	132.4	±	0.9
Hexy acetate	94.9	±	18.7	221.5	±	1.2	158.9	±	19.9	325.5	±	3.9	203.3	±	5.3	233.9	±	2.9
E2-hexenyl acetate	106.6	±	17.0	170.8	±	26.3	90.5	±	18.0	158.0	±	42.5	132.5	±	1.0	161.6	±	0.4
Z3-hexenyl acetate	13.6	±	2.0	27.7	±	9.0	74.7	±	25.4	64.4	±	5.2	33.9	±	6.2	15.4	±	2.7
Methyl acetate	41.3	±	3.5	59.6	±	4.9	2.6	±	0.2	17.3	±	0.3	7.6	±	1.0	22.8	±	1.1
Methyl hexanoate	27.2	±	1.2	29.4	±	0.8	99.6	±	3.1	98.1	±	1.5	55.3	±	1.8	39.3	±	1.9
Ethyl hexanoate	957.8	±	72.6	1398.6	±	96.6	1027.1	±	5.6	483.7	±	25.6	1045.0	±	37.3	939.5	±	296.0
2-Me-butanal	9.5	±	0.9	11.6	±	2.2	41.5	±	5.9	83.0	±	9.6	20.3	±	6.4	24.2	±	1.6
3-Me-butanal	4.5	±	0.4	11.0	±	0.5	11.8	±	2.4	25.5	±	3.7	25.4	±	6.3	22.6	±	0.8
2+3-Methyl-butanol	9.2	±	0.8	16.2	±	2.1	3.6	±	0.4	4.3	±	0.4	3.9	±	0.2	2.6	±	0.2
limonene	13.2	±	13.2	8.2	±	0.4	19.0	±	6.6	13.3	±	2.0	104.9	±	3.8	211.9	±	1.9
β-Ocymene	1921.9	±	398.6	10369.9	±	487.2	1272.5	±	31.2	4881.9	±	101.5	1594.6	±	94.7	1709.7	±	2.1

Table S3. Significant Pearson correlation coefficients ($p \leq 0.05$) between the infestation status and the main volatile compounds found in VOO.

Compound	<i>r</i>
ethyl acetate	0.822
ethanol	0.483
(Z)-hex-3-enal	-0.910
(Z)-hex-2-enal	-0.897
(E)-hex-2-enal	0.753
(E)-hex-3-enol	0.554
(Z)-hex-3-enol	0.553
(E)-hex-2-enol	0.694
hexan-1-ol	0.566
pent-1-en-3-one	-0.902
(Z)-pent-2-enal	-0.927
pent-1-en-3-ol	-0.688
pentan-3-one	0.864
(E)-hex-2-en-1-yl acetate	0.764
(Z)-hex-3-en-1-yl acetate	-0.096
β -ocimene	0.626

Table S4: Statistically significant correlation coefficients between VOO phenolic compounds and infestation by BO

Compounds (ng/g oil)	Correlation Coefficient
Hydroxytyrosol	-0.802598
Tyrosol	-0.856506
Vanillic acid	-0.787263
vanillin	-0.728496
Pinoresinol	-0.744461
Cinnamic acid	-0.831550
Acetoxipinoresinol	-0.915263
3,4-DHPEA-EA	-0.699919
p-HPEA-EA	-0.696055
Ferulic acid	-0.579958
Luteolin	-0.754357
Apigenin	-0.731996

Table S5. Phenolic composition of olive fruits

Phenolic compounds (µg/g FW)	Manzanilla		Picual		Hojiblanca	
	Control	Infested	Control	Infested	Control	Infested
Hydroxytyrosol glucoside	3119,9b	1870,8a	781,6a	1091,5b	3172,5b	2776,1a
Tyrosol glucoside	301,4b	159,4a	67,7a	72,9a	226,7b	199,8a
Demethyl oleuropein	0,0a	0,0a	0,0a	0,0a	191,6a	122,8a
Oleuropein	6817,7a	13917,2b	5607,3a	5305,6a	3280,9a	3223,0a
Comselogoside	2010,7a	2253,9b	3867,9b	1556,5a	646,1a	893,9b
Ligstroside	218,1a	834,0b	390,8b	312,4a	130,9a	136,9a
Verbascoside	1437,5a	3432,7b	1230,5a	2554,4b	3298,9a	3193,6a
Rutin	216,0a	381,3b	593,7b	149,1a	427,7a	390,9a
luteolin-7-glucoside	182,6a	264,8b	60,6a	155,9b	587,2a	547,4a
total	14304,1a	23114,3b	12600,4b	11198,5a	11962,8a	11484,8a

(*) mean contents and standard deviations from three different analyses

(**) different letters within the same olive cultivar indicate statistically significant differences ($p \leq 0.05$)

Table S6. Real Time-Quantitative PCR primers used in this work.

Primer	Sequence (5' → 3')
qOeGLU1A-F	GAAGAACGTCGTAAAAGGCT
qOeGLU1A-R	CAACAATGACATGACTTTTCAACC
qOeGLU1B-F	GAAGAACGTCGTAAAAGGCT
qOeGLU1B-R	GTTGAAACCTCACTGGCCAGGTCTTT
qOePPO1-F	AGTGTA CTGCTGCCGGAAGTTTG
qOePPO1-R	TGTTGATTGGAACCAACCACCT
qOePPO2-F	CGCCTGCTGTTCTTGTCTTCTCA
qOePPO2-R	GTGCAAAGTGCAACCATCGATTA
qOe1LOX2-F	GAGAATTGGGTGCGTTCATAC
qOe1LOX2-R	TCCTCTGGTGTGGCTAATGTC
qOe2LOX2-F	GATCCAAACGACACCGAAAAGGAGGAA
qOe2LOX2-R	GGCATTATATACTTATCATCTTTCCAG
qOeEF1 α -F	TGCTCTATCTGGATTGCCATT
qOeEF1 α -R	TCAAATGCCACCATGACTTC
qOeGAPDH-F	TGAGATGCTGCACAATGGTT
qOeGAPDH-R	CACGATAGGCTTACGCAACA