

Table 3. Identified phytochemicals in palm oils and extra virgin olive oil using LC-MS/MS

Peak	Phytochemicals	t_R (min)	Molecular Formula	Measured mass-to- charge Ratio (m/z), [M-H] ⁺	Mass Error [mDa]	MS/MS Fragments (m/z)	Classification Details	CPPO	Palm Cooking Oil	RPO	EVOO	Ref.
1	Nonanedioic acid (azelaic acid)	10.8	C ₉ H ₁₆ O ₄	187.0992	1.6	169.0894, 125.0970	Dicarboxylic acid, plant signalling metabolite	√	√	√		[24,25]
2	Oxononanoic acid	10.9	C ₉ H ₁₆ O ₃	171.1048	2.1	127.1163	Medium-chain oxo-fatty acid	√				[26,27]
3	Dihydroxy- methoxyflavanone (sakuranetin)	13.3	C ₁₆ H ₁₄ O ₅	285.0794	2.5	165.0209, 119.0463, 93.0296	Methoxyflavanone	√				[28,29]
4	Trihydroxy- octadecenoic acid	13.6	C ₁₈ H ₃₄ O ₅	329.2344	1.0	229.1504, 171.1023	Trihydroxy fatty acid	√				[30,31]
5	Dihydroxy- methoxyflavone (wogonin)	14.2	C ₁₆ H ₁₂ O ₅	283.0637	2.5	268.0405	O-methylated flavone	√				[32,33]
6	Hydroxy- oxooctadecenoic acid	15.3	C ₁₈ H ₃₂ O ₄	311.2254	2.6	293.2152, 211.1358, 171.1043	Plant oxygenated fatty acid, natural hydroperoxide (oxylipin)	√				[37,38,39]
7	Decanoic acid (capric acid)	15.6	C ₁₀ H ₂₀ O ₂	171.1401	1.0	153.1436, 127.0374	Saturated fatty acid	√				[40]
8	Hydroxyoctadecadienoic acid	16.2	C ₁₈ H ₃₂ O ₃	295.2319	4.0	277.2198, 195.1421, 171.1048	Plant oxygenated fatty acid, natural hydroperoxide (oxylipin)	√				[37,38,39]
9	Dodecanoic acid (lauric acid)	16.6	C ₁₂ H ₂₄ O ₂	199.1734	3.0	181.0247	Saturated fatty acid	√				[40]
10	Glyceryldiacetate 2- palmitate	17.1	C ₂₃ H ₄₂ O ₆	413.4420	3.6	59.0117	Diglyceride derivatives	√	√	√		[41,42]
11	Octadecatrienoic acid (linolenic, ALA)	17.5	C ₁₈ H ₃₀ O ₂	277.2145	2.8	233.2288	Polyunsaturated omega-3 fatty acid	√	√	√	√	[41,42]
12	Hexadecenoic acid (palmitoleic, POA)	17.6	C ₁₆ H ₃₀ O ₂	253.2204	3.1	209.1381	Monounsaturated omega-7 fatty acid	√			√	[41,42]
13	Octadecadienoic acid (linoleic, LA)	18.0	C ₁₈ H ₃₂ O ₂	279.2310	1.9	261.2226	Polyunsaturated omega-6 fatty acid	√	√	√	√	[41,42]
14	Hexadecanoic acid (palmitic, PA)	18.4	C ₁₆ H ₃₂ O ₂	255.2307	2.2	211.2005	Saturated fatty acid	√	√	√	√	[41,42]
15	Octadecenoic acid (oleic, OA)	18.6	C ₁₈ H ₃₄ O ₂	281.2466	2.0	237.3641	Monounsaturated omega-9 fatty acid	√	√	√	√	[41,42]
16	Octadecanoic acid (stearic, SA)	19.8	C ₁₈ H ₃₆ O ₂	283.2610	3.3	239.2309	Saturated fatty acid	√	√	√	√	[41,42]

Table 3 (cont'd). Identified phytochemicals in palm oils and extra virgin olive oil using LC-MS/MS

Peak	Phytochemicals	t_R (min)	Molecular Formula	Measured mass-to- charge Ratio (m/z), [M-H] ⁻	Mass Error [mDa]	MS/MS Fragments (m/z)	Classification Details	CPPO	Palm Cooking Oil	RPO	EVOO	Ref.
17	Hydroxytyrosol	5.6	C ₈ H ₁₀ O ₃	153.0567	1.0	123.0454	Phenylethanoid phenolic compound				√	[43,44]
18	Tyrosol	6.8	C ₈ H ₁₀ O ₂	137.0619	1.1	119.0484, 106.0420	Phenylethanoid phenolic compound				√	[44]
19	Elenolic acid	9.7	C ₁₁ H ₁₄ O ₆	241.0726	0.9	165.0736, 139.0079, 127.0422	Phenolic compound				√	[45]
20	Oleaceinic acid	10.1	C ₁₇ H ₂₀ O ₇	335.1160	2.4	181.0520, 155.0716, 111.0836	Phenolic secoiridoids				√	[46]
21	Oleacein	10.1	C ₁₇ H ₂₀ O ₆	319.1187	2.6	275.1028, 249.0820, 183.0694, 165.0572, 69.0333	Phenolic secoiridoids				√	[47,48]
22	Oleocanthalic acid	10.9	C ₁₇ H ₂₀ O ₆	319.1246	1.4	199.0646, 181.0531, 111.0105	Phenolic secoiridoids				√	[46]
23	Oleocanthal	11.1	C ₁₇ H ₂₀ O ₅	303.1243	0.5	285.1155, 217.0054, 183.0693, 165.0605, 141.0183	Phenolic secoiridoids				√	[47,48]
24	Oleuropein aglycone isomer	11.8	C ₁₉ H ₂₂ O ₈	377.1252	1.0	307.0874, 275.0870, 149.0267, 139.0371	Phenolic secoiridoids				√	[49,50]
25	Oleuropein aglycone isomer	12.1	C ₁₉ H ₂₂ O ₈	377.1249	0.7	307.0874, 275.0855, 149.0268, 139.0371	Phenolic secoiridoids				√	[49,50]
26	Ligstroside aglycone	12.5	C ₁₉ H ₂₂ O ₇	361.1304	1.1	291.0920, 259.0954	Phenolic secoiridoids				√	[47,50,51]
27	Ligstroside aglycone	12.8	C ₁₉ H ₂₂ O ₇	361.1329	3.6	291.0924, 259.1012	Phenolic secoiridoids				√	[47,50,51]