

Table S1. Secoiridoids and other phenolic compounds reported in olive tree products and by products*

| No | Phenolic compounds | References | Molecular Mass | Olive Fruit | Olive Pulp/Mesocarp | Olive Seed/Stone | Virgin Olive Oil | Leaves | Olive Pomace | Olive Mill Wastewater, OMW |
|--|--|-------------------------------------|----------------|-------------|---------------------|------------------|------------------|--------|--------------|----------------------------|
| Secoiridoids | | | | | | | | | | |
| Oleuropein and related compounds | | | | | | | | | | |
| 1 | Oleuropein glucoside (di) | [57,65] | 702.2 | | | | | + | | |
| 2 | Methoxy-oleuropein | [57,63] | 570.5 | | | | | + | | |
| 3 | Hydroxy-oleuropein | [63] | 556.2 | | | | | | | |
| 4 | Oleuropein | [56,57,58,59,60,61,62,69, 70,73,75] | 540.5 | + | + | + | | + | + | + |
| 5 | Oleuropein derivative | [63] | 528.2 | | | | | + | | |
| 6 | Demethyl-oleuropein | [56,57,63,73,75,76] | 526.5 | + | + | | | + | | |
| 7 | 10-Hydroxy-oleuropein aglycone | [64] | 396.4 | | | | + | | + | |
| 8 | Oleuropein aglycone oxidized aldehyde and hydroxylic form/carboxylic form of oleuropein aglycone | [60,72] | 394.1 | | | | + | | | |
| 9 | Oleuropein aglycone/3,4-DHPEA-EA | [58,59,61,63,70,73,74,75] | 378.4 | + | | | + | + | + | |
| 10 | Aldehydic form of oleuropein aglycone | [59,60,70] | 377.4 | | | | + | | | |
| 11 | Dialdehydic form of oleuropein aglycone/Oleuropeindial | [60,64,73,74] | 376.4 | | | | + | | | |
| 12 | Enolic tautomer of the dialdehydic form of oleuropein aglycone/Oleomissional | [64,71] | 365.4 | | | | + | | | |
| 13 | Oleuropein aglycone derivative | [63] | 360.1 | | | | | | + | |
| 14 | 10-Hydroxy-decarboxymethyl oleuropein aglycone | [64] | 336.1 | | | | + | | + | + |
| 15 | Decarboxymethyl oleuropein aglycone oxidised dialdehyde form/Oleaceinic acid | [60,69,72] | 336.1 | | | + | + | | | |
| 16 | Dialdehydic form of decarboxymethyl elenolic acid linked to 3,4-DHPEA/Deacetoxy oleuropein aglycone/Oleacein | [59,60,61,63,73,74] | 320.3 | | | | + | | | |
| 17 | Decarboxymethyl (deacetoxy) form of oleuropein aglycone | [64,70,73] | 319.3 | | | | + | | | + |
| Ligstroside and related compounds | | | | | | | | | | |
| 18 | Ligstroside | [56,61,63] | 524.5 | + | + | | | + | | |
| 19 | Ligstroside aglycone oxidized aldehyde and hydroxylic form/carboxylic form of ligstroside aglycone | [60,72] | 378.1 | | | | + | | | |
| 20 | Methyl acetal of ligstroside aglycone | [66–68] | 375.4 | + | | | | | | |
| 21 | Ligstroside aglycone/p-HPEA-EA | [57,59,63,70,73,74,75] | 362.1 | | | | + | + | | |

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|---------------------------|--|------------------------------|-------|---|--|---|---|--|---|---|---|
| 22 | Aldehydic form of ligstroside aglycone/Ligstral | [59,60,70] | 361.4 | | | | + | | + | | + |
| 23 | Dialdehydic form of ligstroside aglycone/Ligstrodial | [60,64,73,74] | 361.4 | | | | + | | + | | |
| 24 | Enolic tautomer of the dialdehydic form of ligstroside aglycone/Oleokoronal | [64,71] | 361.4 | | | | + | | + | | + |
| 25 | Decarboxymethyl ligstroside aglycone oxidised dialdehyde form/Oleocanthalic acid | [60,72] | 320.1 | | | | + | | | | |
| 26 | Decarboxymethyl (deacetoxy) form of ligstroside aglycone | [64,73] | 304.3 | | | | + | | | | |
| 27 | Dialdehydic form of decarboxymethyl elenolic acid linked to p-HPEA/Oleocanthal/Deacetoxy ligstroside aglycone | [59,60,61,63,70,73,74] | 304.3 | | | | + | | + | | |
| Other secoiridoids | | | | | | | | | | | |
| 28 | Nuzhenide oleoside | [56] | 1059 | | | | + | | + | | |
| 29 | Methyl (5E,6S)-5-ethylidene-4-[2-oxo-2-[[[(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(4-hydroxyphenyl)ethoxy]oxan-2-yl]methoxy]ethyl]-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4H-pyran-3-carboxylate/Nuzhenide | [56,61,65] | 686.2 | + | | | + | | + | + | + |
| 30 | Methyl 4-[2-[2-(3,4-dihydroxyphenyl)ethoxy]-2-oxoethyl]-3-ethenyl-2-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-3,4-dihydro-2H-pyran-5-carboxylate/Oleuroside | [56,57,63] | 540.5 | | | | | | + | | |
| Flavonoids | | | | | | | | | | | |
| 31 | Luteolin-7-O-rutinoside | [56,57,58,63,65] | 610.5 | | | | | | + | + | + |
| 32 | Luteolin diglucoside | [57,59,65] | 610.5 | | | | | | + | + | |
| 33 | (2S)-3',5-Dihydroxy-4'-methoxy-7-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranosyloxy]flavan-4-one/Hesperidin/Hesperetin 7-rutinoside | [56, 65] | 610.6 | + | | + | | | + | | |
| 34 | Quercetin rutinoside (3)/Rutin | [56,57,58,61,62,63,65,70,75] | 610.5 | + | | + | | | + | + | + |
| 35 | Cyanidin-3-rutinoside | [66—68] | 595.5 | | | | | | | | |
| 36 | Apigenin diglucoside | [57] | 594.5 | | | | | | + | | |
| | Apigenin rutinoside | [57,63,66—68,70] | 578.5 | + | | + | | | + | + | |
| 37 | (2S,3R,4S,5S,6R)-2-[2-(3,4-Dihydroxyphenyl)-5,7- | [65,75] | 484.8 | + | | + | | | + | | |

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|----------------|---|---------------------------|-------|---|--|---|---|---|---|
| | dihydroxychromenylium-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol/Cyanidin-3-glucoside | | | | | | | | |
| 38 | Diosmetin-7-O-glucoside | [65] | 462.4 | | | | | + | |
| 39 | 5-Hydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]chromen-4-one/Chrysoeriol-7-O-glucoside | [57,63] | 462.4 | | | | | + | |
| 40 | Luteolin-4'-O-glucoside | [63] | 448.4 | | | | | + | + |
| 41 | Luteolin-5-O-glucoside | [61,70] | 448.4 | + | | | | | |
| 42 | Luteolin-7-O-glucoside | [56,58,60,61,63,65,70,75] | 448.4 | + | | + | | + | + |
| 43 | Quercetin-3-rhamnoside | [66–68] | 448.4 | + | | | | | |
| 44 | Apigenin-7-O-glucoside | [56,57,61,63,65,70] | 432.4 | + | | + | | + | |
| 45 | 3,4',5,7-Tetrahydroxy-3'-methoxyflavone/Isorhamnetin | [57] | 316.3 | | | | | | |
| 46 | 4',5-Dihydroxy-6,7-dimethoxyflavone/Cirsimaritin | [65] | 314.3 | | | | | + | |
| 47 | Gallocatechin | [57] | 306.3 | | | | | + | |
| 48 | (2R,3R)-3,3',4',5,7-Pentahydroxyflavan-4-one/Taxifolin | [59,63,70] | 304.3 | | | | + | + | |
| 49 | 3,3',4',5,7-Pentahydroxyflavone/Quercetin | [56,57,58,63] | 302.2 | | | + | | + | + |
| 50 | 5,7,3'-Trihydroxy-4'-methoxyflavone/Diosmetin | [57] | 300.3 | | | | | + | |
| 51 | (2R,3S)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-chromene-3,5,7-triol/Catechin | [57,65] | 290.3 | | | | | + | |
| 52 | 2-(3,4-Dihydroxyphenyl)-5,7-dihydroxychroman-4-one/Eriodictyol | [63] | 288.3 | | | | | + | |
| 53 | 3',4',5,7-tetrahydroxyflavone/Luteolin | [56,57,58,59,61,62,63,65] | 286.2 | | | + | + | + | + |
| 54 | (2S)-4',5,7-Trihydroxyflavan-4-one/Naringenin | [62] | 272.3 | | | | | | + |
| 55 | 4',5,7-trihydroxyflavone/Apigenin | [56,57,58,59,61,63] | 270.3 | | | | + | + | + |
| 56 | Luteolin-hexoside | [63] | 448.1 | | | | | + | + |
| Lignans | | | | | | | | | |
| 57 | 4,4'-[(1R,3aS,4R,6aS)-tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diyl]bis(2,6-dimethoxyphenol)/Syringaresinol | [65] | 418.4 | | | | | + | |
| 58 | [(3R,3aS,6S,6aR)-3,6-bis(4-hydroxy-3-methoxyphenyl)-3,4,6,6a-tetrahydro-1H-furo[3,4-c]furan-3a-yl] acetate/1-Acetoxy-pinorensinol | [58, 60, 62, 69, 74] | 416.4 | | | + | + | + | + |
| 59 | 1-Hydroxy-pinorensinol | [59,70] | 372.4 | | | | | + | |

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| 60 | 4-[(3S,3aR,6S,6aR)-6-(4-Hydroxy-3-methoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenol/Pinoresinol | [58,59,61,63,70,75] | 358.4 | | + | | + | + | + | + | + |
| Phenolic acids | | | | | | | | | | | |
| 61 | <i>p</i> -Coumaroyl-6'-secologanoside/Comselogoside | [62] | 536.2 | | | | | | | | |
| 62 | (1S,3R,4R,5R)-3-[[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy]-1,4,5-trihydroxycyclohexane-1-carboxylic acid/Chlorogenic acid/Caffeoyl-quinic acid | [56,57,60,61,62,63,65,70,75] | 354.3 | + | + | | | + | + | | |
| 63 | (2R,3R)-2-[[(2E)-3-(3,4-Dihydroxyphenyl)prop-2-enoyl]oxy]-3-hydroxybutanedioic acid/Caftaric acid | [65] | 312.2 | | | | | + | | | |
| 64 | (2E)-3-(4-Hydroxy-3,5-dimethoxyphenyl)prop-2-enoic acid/Sinapinic acid | [56,58,59,61,73,75] | 224.2 | + | | | + | | | | + |
| 65 | 4-Hydroxy-3,5-dimethoxybenzoic acid/Syringic acid | [56,57,58,61,65,70,73,74,75] | 198.2 | + | + | | + | + | | | + |
| 66 | 3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid/Ferulic acid | [56,57,59,60,61,62,63,65,70,73,75] | 194.2 | + | + | | + | + | + | | |
| 67 | 3,4-Dimethoxybenzoic acid/Veratric acid | [56,58,63] | 182.2 | | + | | | | | | + |
| 68 | (4-hydroxy-3-methoxyphenyl)acetic acid/Homovanillic acid | [56,59,62,65,73,75] | 182.2 | + | + | | + | + | + | | |
| 69 | 3-(3,4-Dihydroxyphenyl)propanoic acid/Dihydrocaffeic acid | [59,70,75] | 182.2 | + | + | | + | | | | |
| 70 | 3-(3,4-Dihydroxyphenyl)-2-propenoic acid/Caffeic acid | [56,57,58,59,60,61,62,63,65,73,74,75] | 180.2 | + | + | | + | + | + | | + |
| 71 | 3,4,5-Trihydroxybenzoic acid/Gallic acid | [56,57,58,59,60,61,63,64,70,73,74] | 170.1 | + | + | | + | + | + | | + |
| 72 | 4-Hydroxy-3-methoxybenzoic acid/Vanillic acid | [56,57,59,60,61,62,63,70,73,74,75] | 168.2 | + | + | | + | + | + | | + |
| 73 | 3,4-Dihydroxyphenylacetic acid/Homoprotocatechuic acid | [59,70,75] | 168.2 | + | + | | + | | | | |
| 74 | (2E)-3-(3-Hydroxyphenyl)prop-2-enoic acid/m-Coumaric acid | [80] | 164.2 | + | + | | | | | | |
| 75 | (2E)-3-(2-Hydroxyphenyl)prop-2-enoic acid/o-Coumaric acid | [55, 58, 59, 60, 72, 73, 74] | 164.2 | + | + | | + | | | | |
| 76 | (2E)-3-(4-Hydroxyphenyl)prop-2-enoic acid/p-Coumaric acid | [56,57,58,59,60,61,62,63,73,74,75] | 164.2 | + | + | | + | + | + | | + |
| 77 | 2,5-Dihydroxy benzoic acid/Gentisic acid | [59,73] | 154.1 | | | | + | | | | |
| 78 | 2,4-Dihydroxy benzoic acid/ β -Resorcylic acid | [70] | 154.1 | | | | | | | | |

[illegible]

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|----------------------------|--|------------------|-------|---|---|---|---|---|
| 99 | 3,4-Dihydroxyphenylglycol/4-(1,2-dihydroxyethyl)benzene-1,2-diol | [58,62,63,70,75] | 170.2 | + | | | + | + |
| 100 | 4-Hydroxy-3-methoxybenzaldehyde/Vanillin | [57,65,74] | 152.2 | | + | + | + | + |
| 101 | Benzene-1,2-diol/Catechol | [58] | 110.1 | | | | | + |
| Hydroxy-isochromans | | | | | | | | |
| 102 | 1-(3'-Methoxy-4'-hydroxy)phenyl-6,7-dihydroxyisochroman | [59,7] | 288.3 | | + | | | |
| 103 | 1-Phenyl-6,7-dihydroxyisochroman | [59,70] | 242.3 | | + | | | |

*Within each category compounds 1-103 are presented on descending molecular mass order