

Supplementary Table S1. Parameters for identification of bioactive compounds in olive-tree materials.

Compound name	R _t	Formula	Precursor ion (<i>m/z</i>)	Main product ions (<i>m/z</i>)	Priority samples
Secoiridoids					
Oleuropein ^a	12.15	C ₂₅ H ₃₂ O ₁₃	539.176	507.2762; 225.0747; 112.9845	Leaves
Oleuropein glucoside	11.37	C ₃₁ H ₄₂ O ₁₈	701.2285	539.1776; 275.0893; 153.0529	Leaves
Oleuropein quinone	12.41	C ₂₅ H ₃₀ O ₁₃	537.1612	223.0601; 151.0396; 110.1298	Leaves
Ligstroside	13.05	C ₂₅ H ₃₂ O ₁₂	523.1813	291.0846; 259.0948; 137.0594	Leaves and olive pomace
Hydroxyoleuropein	10.70	C ₂₅ H ₃₂ O ₁₄	555.1709	537.1597; 291.0864; 151.0380	Leaves
Oleacein ^a	12.39	C ₁₇ H ₂₀ O ₆	319.1175	153.0440; 69.0341; 59.0129	Leaves and olive pomace
Oleaceinic acid	10.49	C ₁₇ H ₁₉ O ₇	335.1113	199.0631; 181.0715; 151.0385	Olive pomace
Oleocanthal ^a	13.49	C ₁₇ H ₂₀ O ₅	303.1228	181.0051; 137.0585; 69.0331	Olive pomace
Oleocanthalic acid	12.61	C ₁₇ H ₂₀ O ₆	319.1185	183.0654; 139.0745; 69.0343	Olive pomace
Oleuropein aglycone ^a	14.11	C ₁₉ H ₂₂ O ₈	377.1233	275.0556; 153.0494; 59.0128	Leaves
Oleuropein aglycone quinone	14.01	C ₁₉ H ₂₀ O ₈	375.1095	275.0553; 153.0560; 59.0128	Olive pomace
Ligstroside aglycone ^a	14.59	C ₁₉ H ₂₂ O ₇	361.1282	291.0870; 139.0402; 111.0072	Olive pomace
2-methoxyoleuropein	12.48	C ₂₆ H ₃₄ O ₁₄	569.1874	537.1590; 403.1233; 151.0386	Olive pomace
Demethyloleuropein aglycon	12.93	C ₁₈ H ₂₀ O ₈	363.1085	229.1074; 121.0666; 59.0123	Leaves
Hydroxyoleuropein aglycon	12.27	C ₁₉ H ₂₂ O ₉	393.1182	291.0503; 151.0399; 62.9845	Olive pomace
GL3 ^a	12.14	C ₄₈ H ₆₄ O ₂₇	1071.356	909.3060; 685.2386; 101.0248	Olive pomace
Nuzhenide ^a	12.81	C ₃₁ H ₄₂ O ₁₇	685.2338	685.2447; 453.1346; 101.0232	Olive pomace

Hydroxylated form of decarboxymethyl oleuropein aglycone	10.49	C ₁₇ H ₂₀ O ₇	335.1124	202.9119; 151.03770; 69.0350	Olive pomace
Simple phenols					
3-methylcatechol ^a	9.42	C ₇ H ₈ O ₂	123.0441	95.0479; 69.0329; 41.0015	Leaves and olive pomace
Hydroxytyrosol ^a	9.43	C ₈ H ₁₀ O ₃	153.0544	123.0444; 93.0329; 44.9976	Leaves and olive pomace
Hydroxytyrosol glucoside	8.89	C ₁₄ H ₂₀ O ₈	315.1072	153.0537; 123.0442; 59.0129	Olive pomace and leaves
Hydroxytyrosol-lathyroside	8.99	C ₁₉ H ₂₈ O ₁₂	447.1491	315.888; 153.0548; 44.9976	Leaves and olive pomace
Tyrosol acetate	10.48	C ₁₀ H ₁₂ O ₃	179.0705	137.3739; 123.0421; 68.9950	Olive pomace and olive
Flavonoids					
Apigenin ^a	14.49	C ₁₅ H ₁₀ O ₅	269.0441	225.0538; 151.0028; 117.0333	Leaves
Luteolin ^a	13.92	C ₁₅ H ₁₀ O ₆	285.0395	199.0389; 175.0396; 151.0033	Leaves
Luteolin-7-O-glucoside ^a	12.69	C ₂₁ H ₂₀ O ₁₁	447.0921	327.0486; 285.0405; 167.0329	Leaves
Luteolin-7-rutinoside ^a	10.90	C ₂₇ H ₃₀ O ₁₅	593.1505	285.0402; 151.9935; 137.8169	Leaves
Quercitrin ^a	12.26	C ₂₁ H ₂₀ O ₁₁	447.0920	300.0264; 254.9830; 151.0364	Leaves
Quercetin-3-glucoside ^a	11.46	C ₂₁ H ₂₀ O ₁₂	463.0875	424.4496; 300.0259; 190.9303	Leaves
Rhoifolin ^a	11.54	C ₂₇ H ₃₀ O ₁₄	577.1526	269.0449; 151.0037; 112.9837	Leaves
Rutin ^a	11.14	C ₂₇ H ₃₀ O ₁₆	609.1456	385.1314; 301.0322; 151.0041	Leaves
Triterpenes					
Maslinic acid ^a	16.67	C ₃₀ H ₄₈ O ₄	471.3469	392.9793; 266.9875; 118.9934	Olive pomace, leaves and olive
Oleanolic acid	17.51	C ₃₀ H ₄₈ O ₃	455.3524	396.9865; 187.0260; 112.9804	Leaves

R_t, Retention time.

^aConfirmed by analytical standard.