

Supplementary Materials: Antiulcer Potential of *Olea europea* L. cv. Arbequina Leaf Extract Supported by Metabolic Profiling and Molecular Docking

Arafa Musa ^{1,2,*†}, Nourhan Hisham Shady ^{3,†}, Shaimaa R. Ahmed ^{4,5}, Taghreed S. Alnusaire ⁶, Ahmed M. Sayed ⁷, Bassam F. Alowaiesh ^{6,8}, Ibrahim Sabouni ⁸, Mohammad M. Al-Sanea ⁹, Ehab M. Mostafa ^{1,2}, Khayrya A. Youssif ¹⁰, Dalia H. Abu-Baih ¹¹, Mahmoud A. Elrehany ^{11,12} and Usama Ramadan Abdelmohsen ^{3,13,*}

- ¹ Pharmacognosy Department, College of Pharmacy, Jouf University, Sakaka, Aljouf 72341, Saudi Arabia; akmusa@ju.edu.sa
- ² Department of Pharmacognosy, Faculty of Pharmacy, Al-Azhar University, Cairo 11371, Egypt
- ³ Department of Pharmacognosy, Faculty of Pharmacy, Deraya University, New Minia City, Minia 61111, Egypt; Norhan.shady@deraya.edu.eg
- ⁴ Department of Pharmacognosy, Faculty of Pharmacy, Cairo University, Kasr El-Aini Street, Cairo 11562, Egypt; shaimaa.ahmed@pharma.cu.edu.eg
- ⁵ Department of Pharmacognosy, College of Pharmacy, Jouf University, Sakaka, Aljouf 2014, Saudi Arabia
- ⁶ Biology Department, College of Science, Jouf University, Sakaka, Aljouf 72341, Saudi Arabia; tasalnosairi@ju.edu.sa (T.S.A.); bfalawish@ju.edu.sa (B.F.A.)
- ⁷ Department of Pharmacognosy, Faculty of Pharmacy, Nahda University, Beni-Suef 62513, Egypt; Ahmed.mohamed.sayed@nub.edu.eg
- ⁸ Olive Research Center, Jouf University, Sakaka, Aljouf 72341, Saudi Arabia; ibrahimsabouni@gmail.com
- ⁹ Pharmaceutical Chemistry Department, College of Pharmacy, Jouf University, Sakaka, Aljouf 72341, Saudi Arabia; mmalsanea@ju.edu.sa
- ¹⁰ Department of Pharmacognosy, Faculty of Pharmacy, Modern University for Technology and Information, Cairo 11371, Egypt; Khayrya.youssif@pharm.mti.edu.eg
- ¹¹ Department of Biochemistry and molecular biology, Faculty of Pharmacy, Deraya University, New Minia City, Minia 61111, Egypt; Dalia.hamdy@deraya.edu.eg (D.H.A.-B.); Mahmoud.elrehany@deraya.edu.eg (M.A.E.)
- ¹² Department of Biochemistry, Faculty of Medicine, Minia University, Minia 61519, Egypt
- ¹³ Department of Pharmacognosy, Faculty of Pharmacy, Minia University, Minia 61519, Egypt
- * Correspondence: akmusa@ju.edu.sa (A.M.); usama.ramadan@mu.edu.eg (U.R.A.)
- † Those authors have equally contributed.

Table S1. Dereplicated metabolites from LC-HRESIMS analysis of *Olea europea* L. cv. Arbequina extract.

Number	<i>m/z</i>	Name of structure	Retention time (RT)	Exact mass	Molecular formula	Peak Area
1	455.352	3-Hydroxy-12-oleanen-28-oic acid; 3β-form	11.10857	456.3592	C ₃₀ H ₄₈ O ₃	1911.6799
2	471.34715	2,3-Dihydroxy-13(18)- oleanen-28-oic acid; (2α,3β)- form	8.92862	472.354	C ₃₀ H ₄₈ O ₄	56903.08

3	539.17654	Oleuropein	2.8017333	540.1838	C ₂₅ H ₃₂ O ₁₃	1975663.5
4	153.05418	2-(3,4-Dihydroxyphenyl) ethanol	2.9556967	154.0629	C ₈ H ₁₀ O ₃	221.12705
5	507.23793	Oliverixanthone	13.451083	508.2452	C ₃₀ H ₃₆ O ₇	1.6716347
6	153.05436	Cleroidicin F	12.28353	154.063	C ₈ H ₁₀ O ₃	25685.429
7	553.19194	Oleuropein; 3"-Me ether	3.5709733	554.1992	C ₂₆ H ₃₄ O ₁₃	1064936.8
8	557.223	Oleoside; 6'-O-(8-Hydroxy- 2,6-dimethyl-2E-octenoyl)	2.6187433	558.2302	C ₂₆ H ₃₈ O ₁₃	1.0510785
9	279.2321	11-Octadecen-9-ynoic acid; (E)-form	11.044853	278.224	C ₁₈ H ₃₀ O ₂	183466.78
Number	<i>m/z</i>	Name of structure	Retention time (RT)	Exact mass	Molecular formula	Concentration
10	455.35185	3-Hydroxy-12-ursen-28-oic acid; 3β-form, 3-Ketone	10.0559	454.3445	C ₃₀ H ₄₆ O ₃	363.18763
11	377.18056	8-Epimer, (3,4- dihydroxyphenylethyl) ester	3.3180933	378.13147	C ₁₉ H ₂₂ O ₈	458.15578
12	439.15729	Chebulic acid 4,5- Didehydro(E-), tri-Et ester	2.9747767	438.156215	C ₂₀ H ₂₂ O ₁₁	1.8959597
13	623.59191	Verbascoside	8.99936	624.592	C ₂₉ H ₃₆ O ₁₅	184019.11
14	285.03958	Luteolin	4.4696567	286.047	C ₁₅ H ₁₀ O ₆	1.2564833
15	225.11194	Olenoside A	3.0286567	226.119	C ₁₁ H ₁₄ O ₅	115.7028
16	317.06576	Olivin	4.3482767	316.05469	C ₁₇ H ₁₆ O ₆	1.4666315
17	203.17977	Olivacene	8.5318633	202.172	C ₁₅ H ₂₂	2008631.1

18	319.11732	Oleacein	9.00507	320.1259	C ₁₇ H ₂₀ O ₆	0.5145
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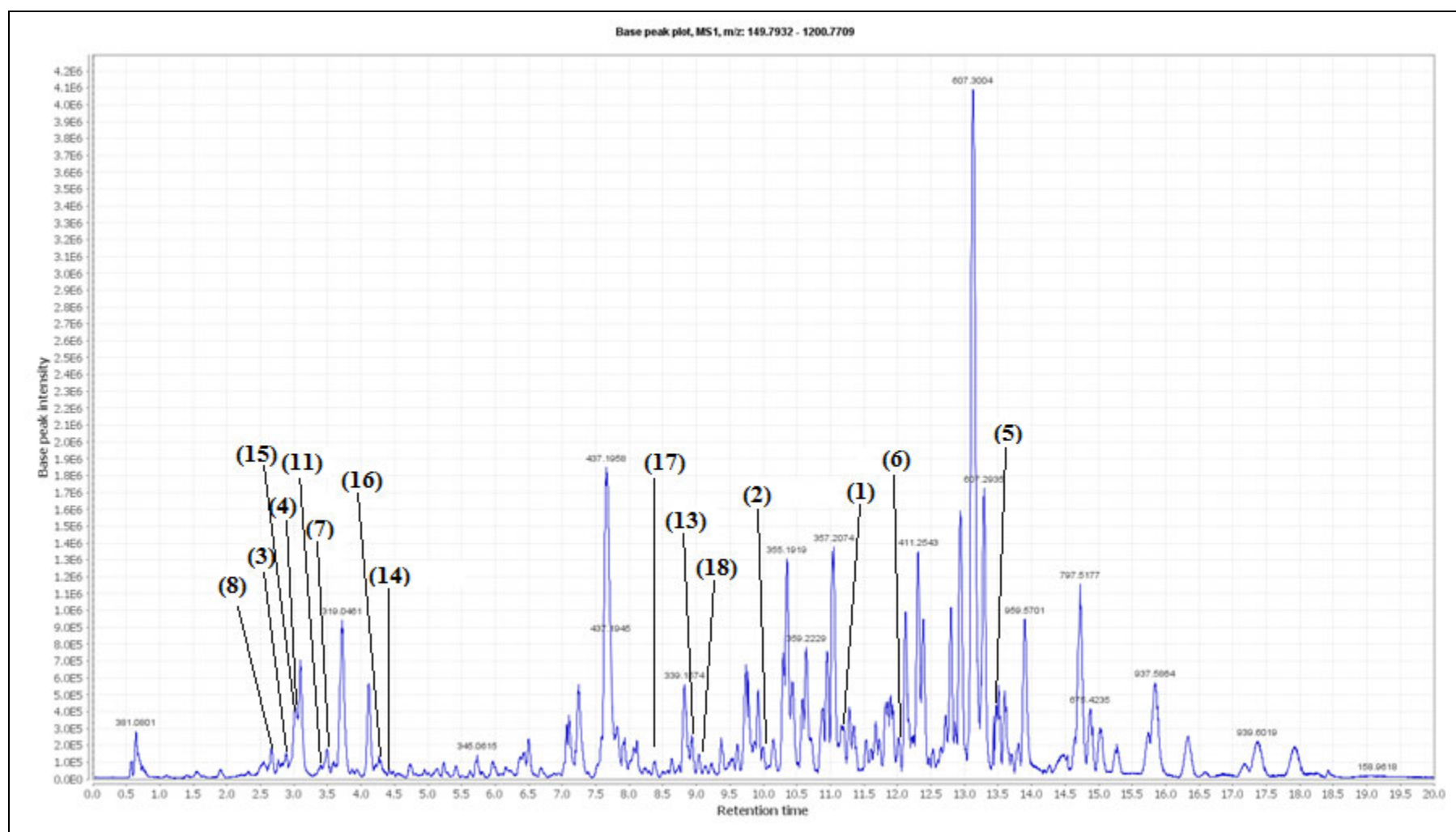


Figure S1. LC-HRESIMS Chromatogram of the putatively dereplicated metabolites of *Olea europaea* L. cv. Arbequina (Negative mode).

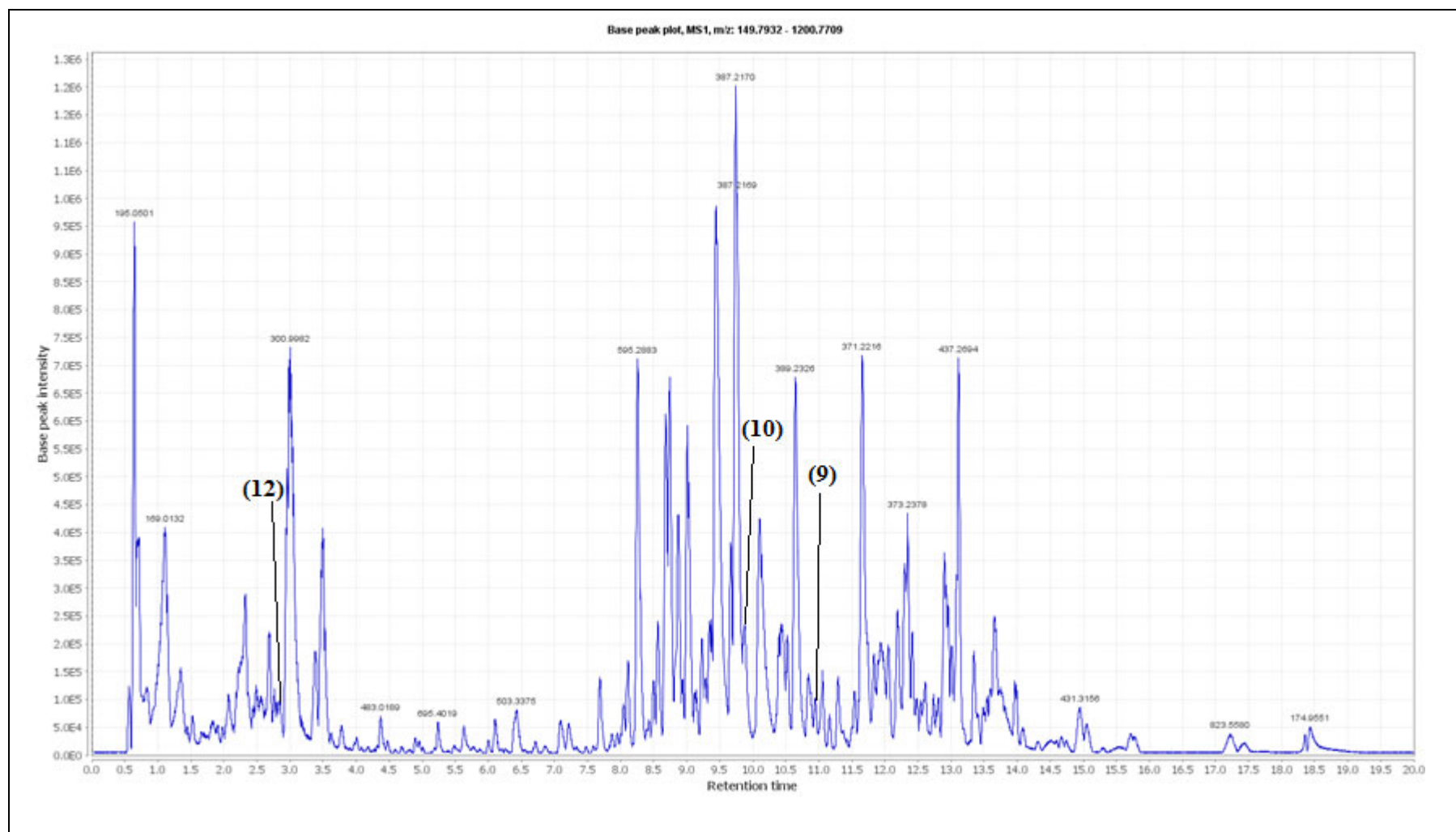


Figure S2. LC-HRESIMS Chromatogram of the putatively dereplicated metabolites of *Olea europaea* L. cv. Arbequina (Positive mode).