A Comparative LC/MS Analysis of Jordanian Olive Stone, Fruits, Leaves, and Oils

NAWAL H. BAHTITI[1,2]*, FATEN M. ABU ORABI[2,3], MOHAMMED H. KAILANI[4], IBRAHIM ABDEL-RAHMAN[5], AYSSAR NAHLÉ[5], ZAHRA O. ALFAOURI[4], HIND H. AL ABDALLAT[4]

[1]Faculty of Arts and Science,
Applied Science Private University,
JORDAN

[2]Middle East University,
Middle East Research Unit,
JORDAN

[3]Department of Chemistry, Faculty of Arts and Science,
Applied Science Private University,
Amman 11931,
JORDAN

[4]Department of Chemistry, Faculty of Science,
The University of Jordan,
Amman 11942,
JORDAN

[5]Chemistry Department, College of Sciences,
University of Sharjah,
P.O. Box: 27272,
UAE

Abstract: - The olive (Oleo europaea L.) may be a broadly dispersed plant that began within the Mediterranean locale. Its natural product is commonly utilized to create olive oil, table olives, and other by-products. Olives are rich in carbohydrates, vitamins, and minerals. Most olive items and the dietary composition of olive oil centering on fatty acids, phenolic compounds, and other cancer prevention agents are changed in numerous parts of olive plants. The most chemical constituents important to the natural movement of olive oil were inspected. Fluid-chromatography–mass spectrometry(LC/MS) investigation uncovered more than 50 major phenolic compounds among which oleuropein, hydroxytyrosol apigenin 7-O-glucoside, tyrosol, catechin, and vanillic corrosive were recognized. Olive clears out, wealthy in carotenoids and chlorophyll, the olive stone and seed are vital products produced within the olive oil extraction, as a lingo cellulosic fabric, the hemicellulose, cellulose, and lignin are the most components of olive stone as well as protein, fat, phenols, free sugars, and polyols composition. Both lipophilic and hydrophilic phenolics are conveyed in olive natural products. The most lipophilic phenols are cresols whereas the major hydrophilic phenols incorporate phenolic acids, phenolic alcohols, flavonoids, and secoiridoids; they are shown in nearly all parts of the plant, but their nature and concentration shift incredibly between the tissues. Olive oil is composed primarily of triacylglycerols (triglycerides or fats) and contains little amounts of free greasy acids (FFA), glycerol, phosphatides, shades, flavor compounds, sterols, and minuscule bits of olive. Olive stones have a most noteworthy sum of rutin. Luteolin appeared the most noteworthy sum in takes off, while the least level was found in oils, tall concentrations of tyrosol, vanillic, and caffeic corrosive, and vanillin was found in stones. In common, rutin and luteolin 7-O-glucoside were the two fundamental flavonoids identified in all parts.

Key-Words: - Olives-Oils, Stone, Leaves, Fruit, chemical composition, LC/MS-analysis.

Received: April 12, 2023. Revised: July 4, 2023. Accepted: September 2, 2023. Published: September 20, 2023.

1 Introduction

The olive tree, or Olea europaea L., is a drought-tolerant plant, [1], that is primarily indigenous to the Mediterranean region, [2]. The olive tree's leaves are easily accessible from the olive grove or from the leftovers of industrial byproducts and agricultural waste, [3], [4]. During pruning, the weight of leaf by-products makes up roughly 25% of the total weight of the pruned residue, depending on geographic variations, horticultural practices, and tree lifetime, [5]. Olive fruit's average composition includes water (50%), protein (1.6%), oil (22%), carbohydrate (19.1%), cellulose (5.8%), inorganic substances (1.5%), and phenolic compounds (1–3%). Other important compounds present in olive fruit are pectin, organic acids, and pigments, [6]. Currently, the main commercial uses of olive leaves are in animal feed, [7], folk medicine, [8], and protection against chronic illnesses like diabetes and cardiovascular disease, [8]. Recent research has focused on uncovering additional applications for olive leaves across a variety of industrial fields, including food, modern medicine, and pharmaceuticals, [9]. Studies have shown that the biological activity of the aglycone portion (aglycones bound to glycones) is greater than that of the glycoside portion, [10]. Olive leaves are abundant in a range of known phenolic groups that are broadly clustered into (*i*) secoiridoids (including oleuropein and oleuropein-aglycone), (*ii*) flavonoids (such as rutin and luteolin-7-glucoside), and (*iii*) simple phenols (such as Hydroxytyrosol and tyrosol. Among the most typical phenolics in olive leaves include hydroxytyrosol, tyrosol, rutin, and oleuropein, [8]. Indeed, oleuropein and hydroxytyrosol are detectably prominent in olive leaves. In their research on evaluating the antioxidant ability of olive leaves from the Tunisian cultivar, they found that oleuropein (6.8 g/100 g fresh leaves) was the principal phenolic constituent in the leaves of olive trees. The protective attributes of oleuropein are reflected typically by their inhibiting effects against (*i*) oxidation, [11], (*ii*) microbial disorders, [11], (*iii*) inflammation, [11], and (*iv*) platelet aggregation, [11]. In addition, oleuropein is found to be effectively capable of re-building the tissue damage, caused by cisplatin in stomach and lung organs, [11]. It's important to note that the phenolic content of olive drupes is comparable to that of olive leaves, [12], but that the proportion adversely decreases during maturation and processing. For instance, likely, processing will significantly deplete oleuropein, especially through enzymatic reactions, [13]. Olive leaves are also valued for their dietary applications because they are abundant in flavonoids. Flavonoids have positive protective effects against infectious, [14], cardiovascular, [14], and cancerous, [14], diseases. One of the most common simple phenolic alcohols is hydroxytyrosol, which is primarily found in olive leaves, [15]. The formation of hydroxytyrosol derives from the hydrolysis of oleuropein, and their numbers grow through (*i*) the stage of maturity, (*ii*) the processing line, [16], and (*iii*) metabolism of oleuropein upon intake of oleuropein-based foods, [17]. Tyrosol, a group of phenolic alcohols, is usually present in a trace amount in olive leaves, [18]. Due to its chemical stability, it is less prone to be degraded by auto-oxidation, [19]. Triterpenoids, namely triterpenes, [20], are the secondary metabolites abundantly found in the waxes/outer coating of leaves, [21]. Olive leaves contain a considerable amount of pent acyclic triterpenoids, with oleanolic acid being the prevailing component ranging from 3.0 to 3.5% up to 3.98% dry basis, [22]. Triterpene-rich olive leaves, with the presence of oleanolic acid and avail, have been found to exhibit suppression against diabetes and inflammatory diseases, [23]. The presence of tocopherols in most lipid-based foods such as olive seeds and vegetable oils is paramount, mainly because of the protective action exerted by tocopherols to inhibit activities of reactive oxygen species such as peroxides, [24], which in turn assists in the prevention of lipid peroxidation in the food, [25]. Chlorophylls and carotenoids, the pigments prevalent in olive pulp, [26], are valued for their color attributes, and functional properties, [27]. Carotenoids, the hydrophobic (fat-soluble) compounds, signify the yelreddish-orangeange color of the cell membranes, [28]. Incorporation of pigment-rich olive leaves in olive oil which are reportedly effective in promoting the nutritional

quality of the oil, [29]. This research describes a novel method of analyzing different chemical compositions of Jordanian olives plants, to evaluate each part.

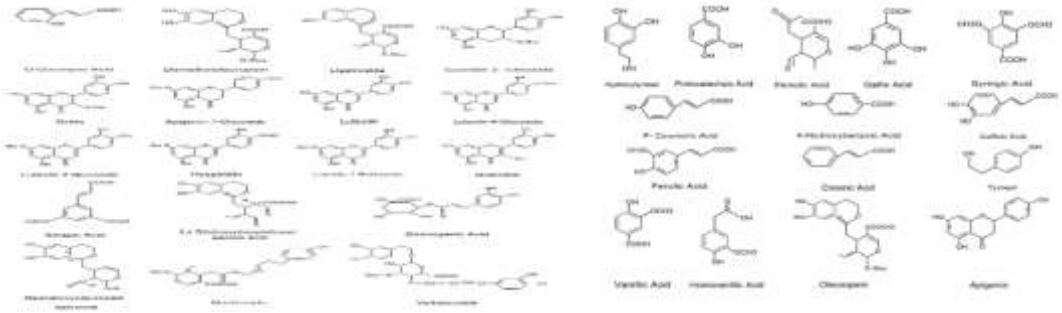

Fig. 1: Chemical Structures of Olives Components.

2 Materials and Methods

2.1 Plant Experimental Method

Stock solutions were prepared by dissolving the appropriate amount of substance in Dimethyl sulfoxide (DMSO), analytical grade, then diluted with acetonitrile and used for identification using the LC/MS technique. The reagents, acetonitrile, methanol, water, and formic acid were LC/MS grade.

2.2 Instrumentation and LC/MS Parameters

A Bruker Daltonik (Bremen, Germany) Impact II ESI-Q-TOF System equipped with Bruker Daltonik Elute UPLC system (Bremen, Germany) was used for screening compounds of interest. Standards for identification of m/z with high-resolution Bruker TOF MS and the exact retention time of each analyte after chromatographic separation were used. This instrument was operated using the Ion Source Apollo II ion Funnel electrospray source. The capillary voltage was 2500 V, the nebulizer gas was 2.0 bar, the dry gas (nitrogen) flow was 8 L/min, and the dry temperature was 200 ºC. The mass accuracy was < 1 ppm; the mass resolution was 50000 FSR (Full Sensitivity Resolution) and the TOF repetition rate was up to 20 kHz. using Elute UHPLC coupled to a Bruker impact II QTOFMS. Chromatographic separation was performed using Bruker solo 2.0_C-18 UHPLC column (100 mm x 2.1 mm x 2.0 µm) at a flow rate of 0.51 mL/min and a column temperature of 40C. Solvents: (A) water with 0.05 % formic acid and (B) acetonitrile. Gradient: 0 – 27 min linear gradient from 5 % - 80 % B; 27 – 29 min 95 % B; 29.1 min 5 % B, total analysis time was 35 min on positive and 35 min on negative mode; injection volume was 3 uL.

3 Results and Discussion

The chemical structures of olives constituents are shown in Figure 1.

All the constituents of olive oil, olive leaves, olive stone, olive branch, and olive fruit are listed in Table 1 (Appendix). Liquid chromatography–mass spectrometry (LC/MS) analysis revealed more than 50 major phenolic compounds some of them shown in Figure 2, Figure 3, Figure 4, Figure 5, Figure 6, Figure 7, Figure 8, Figure 9, Figure 10, Figure 11, Figure 12, Figure 13 and Figure 14, among which oleuropein in Figure 9 and Figure 12, hydroxytyrosol apigenin 7-O-glucoside as in Figure 2, tyrosol, catechin as in Figure 8, and vanillic acid were identified. Olive leaves, rich in carotenoids as in Figure 3 and chlorophyll, the olive stone and seed are important byproducts generated in olive oil extraction, as a lingo cellulosic material, the hemicellulose, cellulose, and lignin as in Figure 11 are the main components of olive stone as well as protein, fat, phenols, free sugars and polyols composition. Both lipophilic and hydrophilic phenolics are distributed in olive fruit. The main lipophilic phenols are cresols while the major hydrophilic phenols include phenolic acids as in Figure 4, Figure 5, Figure 6 and Figure 7, phenolic alcohols, flavonoids, and secoiridoids; as in Figure 3, they are present in almost all parts of the plant, but their nature and concentration vary greatly between the tissues. Olive oil is composed mainly of triacylglycerols (triglycerides or fats) and contains

small quantities of free fatty acids (FFA), glycerol, phosphatides, pigments, flavor compounds, sterols, and microscopic bits of olive. Olive stones have the highest amount of rutin as in Figure 13. Luteolin (Figure 10)showed the highest amount in leaves, whereas the lowest level was found in oils, high concentrations of tyrosol, vanillic, and caffeic acid, and vanillin was found in stones. In general, rutin and luteolin 7-*O*-glucoside (Figure 10) were the two main flavonoids detected in all parts.

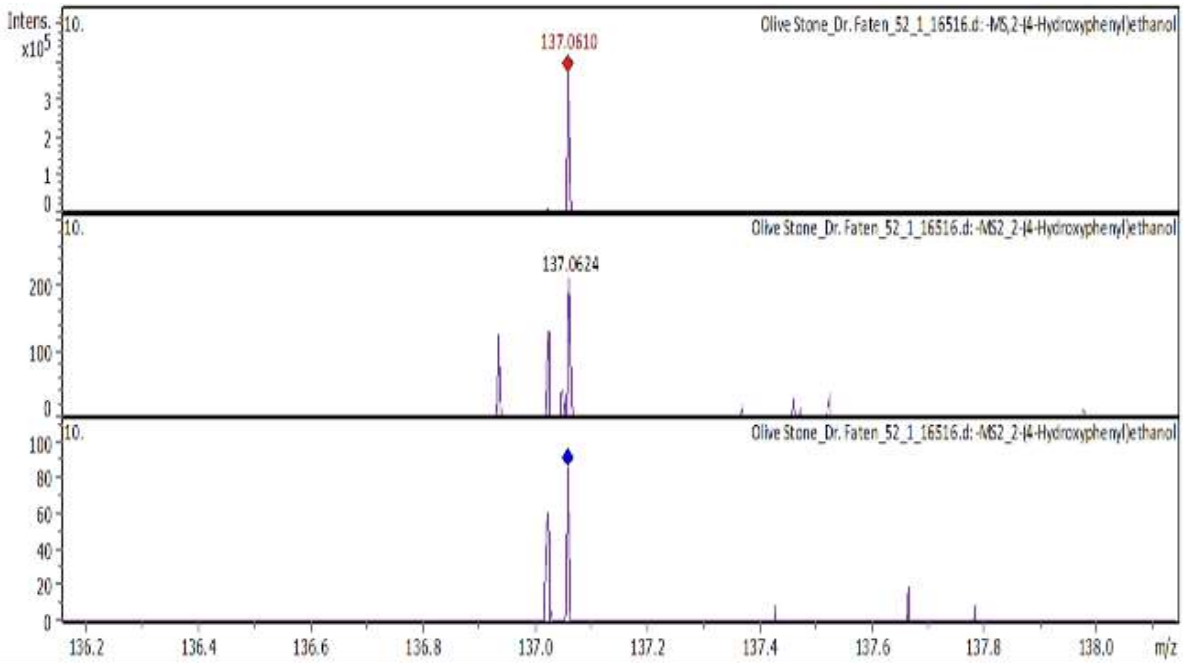

Fig. 2: Constructed LC/MS Chromatography 2,4 hydroxyphenyl ethanol

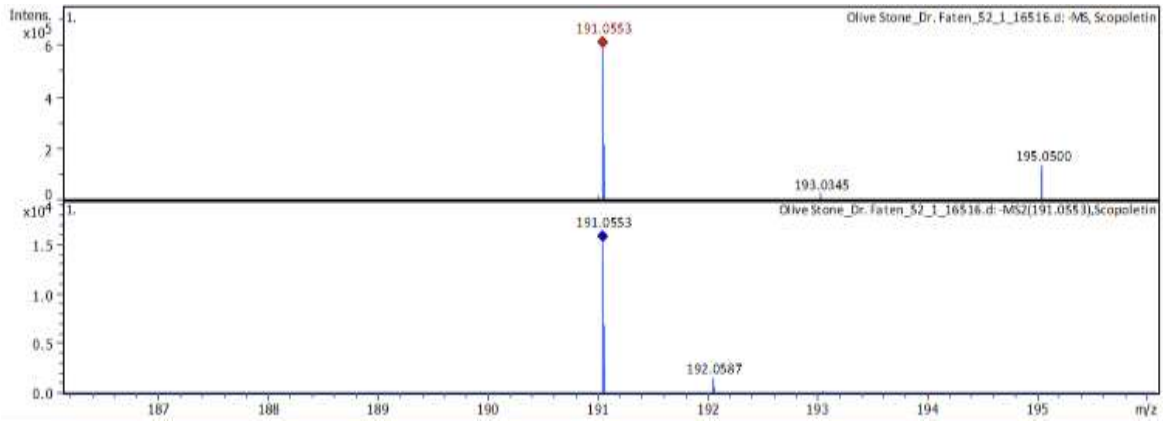

Fig. 3: Constructed LC/MS chromatography of Scopoletin

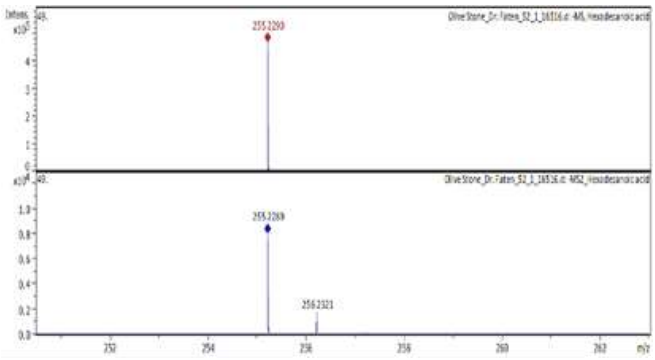

Fig. 4. Constructed LC/MS chromatography hexadecanoic acid

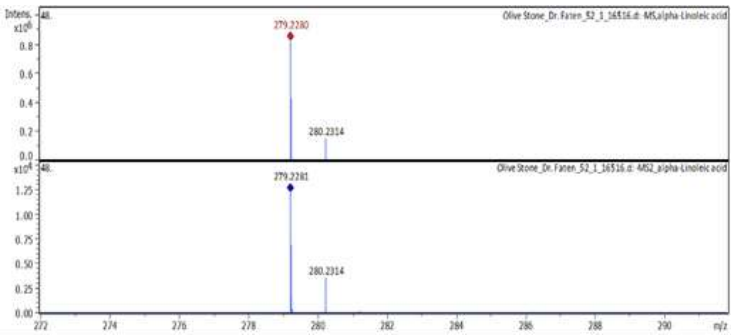

Fig. 5: Constructed LC/MS chromatography ms, alpha-linoleic acid

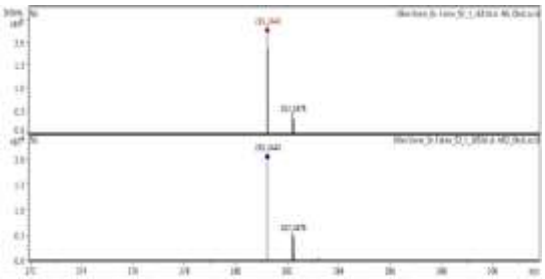

Fig. 6: Constructed LC/MS chromatography of oleic acid

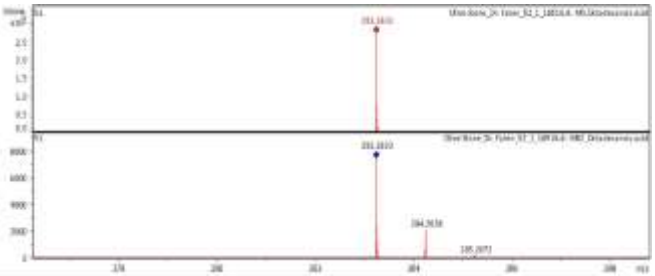

Fig. 7: Constructed LC/MS chromatography of oladecanoic acid

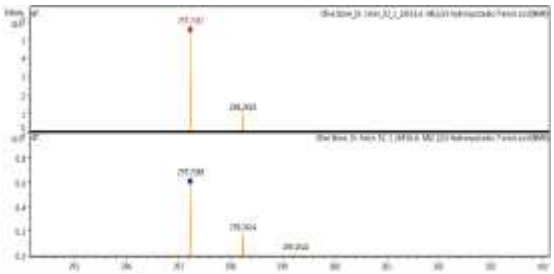

Fig. 8: Constructed LC/MS chromatography 2-3 hydroxyoctaenoic acid

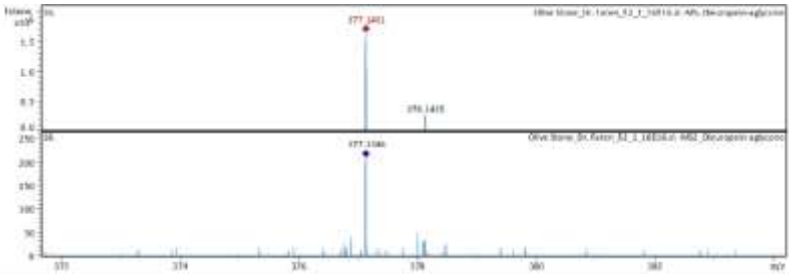

Fig. 9: Constructed LC/MS chromatography oleuropein aglycone

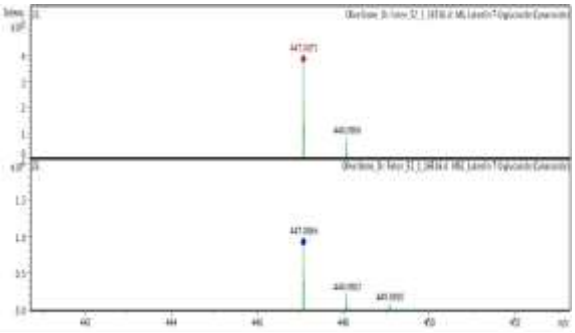

Fig. 10: Constructed LC/MS chromatography Luteolin 7-glucoside

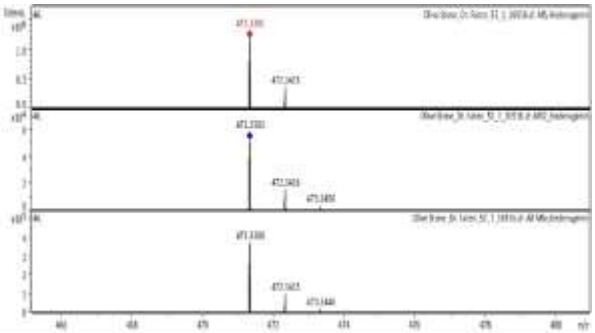

Fig. 11: Constructed LC/MS chromatography Hederagenin

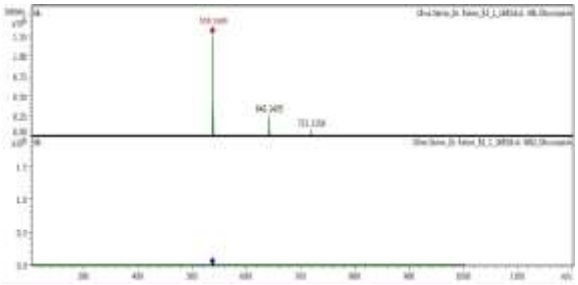

Fig. 12: Constructed LC/MS chromatography oleuropein

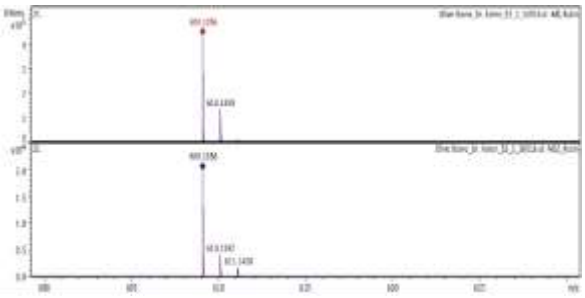

Fig. 13: Constructed LC/MS chromatography rutin

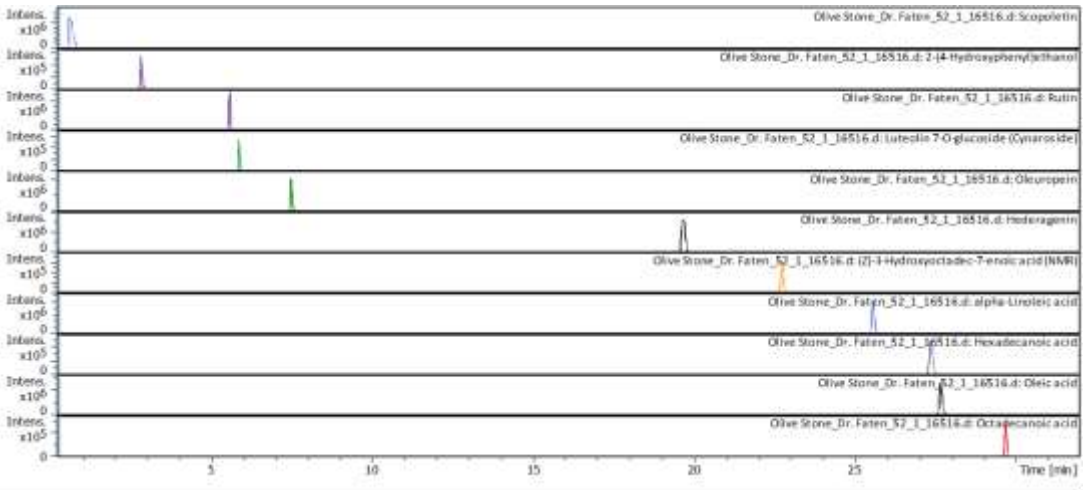

Fig. 14: Example outcome plot from LC-MS analysis of Olive stone

4 Conclusion

This research presents the assortment of chemical composition of all parts of olives. Each part of the olive fruit has a special use of its useful materials for humans. The chemometric elaborations of the information from phenolic profiles picked up by LC-MS/MS permitted us to recognize and segregate between the different olive cultivars examined. The inquiry appears that the subjective and quantitative profile of all distinguished phenolic compounds can be utilized in profundity classifying Jordanian olives cultivars. In conclusion, the application of the LC–MS/Ms procedure for the investigation of virgin olive oil permitted the location of noteworthy contrasts within the extent of constituents from oils of diverse parts of olives. All the oils delivered and analyzed appeared exceptionally high values for the phenolic corrosive (Quinic corrosive; ferulic corrosive; and o-coumaric acids); a higher concentration of decarboximethylated determined of oleuropein aglycon.

Acknowledgements:
The authors acknowledge Applied Science Private University, Amman, Jordan, for the full financial support granted to this research article. Sincere thanks to all my Colleagues in the basic science department, for creating inspiring conditions for work.

References:

[1] Zebin Guo, Xiangze Jia, and Zhichang Zheng Chemical composition and nutritional function of olive (Olea europaea L.): a review October 2018 Photochemistry Reviews 17(7055) DOI: 10.1007/s11101-017-9526-0.

[2] Kabbash, E. M., T., Z., H., S., Wink, M., & Ayoub, I. Comparative metabolic profiling of olive leaf extracts from twelve different cultivars collected in both fruiting and flowering seasons. *Scientific Reports*, *13*(1),

p.1-13. (2023). https://doi.org/10.1038/s41598-022-27119-5.

[3] Artajo, L. S., Romero, M. P., Morelló, J. R. & Motilva, M. J. Enrichment of refined olive oil with phenolic compounds: Evaluation of their antioxidant activity and their effect on the bitter index. *J. Agric. Food Chem.* 54, p.6079–6088 (2006).

[4] Pasković I, Lukić I, Žurga P, Majetić Germek V, Brkljača M, Koprivnjak O, Major N, Grozić K, Franić M, Ban D, Marcelić Š, Goreta Ban S. Temporal Variation of Phenolic and Mineral Composition in Olive Leaves Is Cultivar Dependent. Plants (Basel). 2020 Aug 27;9(9):1099. doi: 10.3390/plants9091099. PMID: 32867040; PMCID: PMC7570285.

[5] Olmo-García L, Bajoub A, Benlamaalam S, Hurtado-Fernández E, Bagur-González MG, Chigr M, Mbarki M, Fernández-Gutiérrez A, Carrasco-Pancorbo A. Establishing the Phenolic Composition of *Olea europaea* L. Leaves from Cultivars Grown in Morocco as a Crucial Step Towards Their Subsequent Exploitation. Molecules. 2018 Oct 2;23(10): 2524.doi: 10.3390/molecules23102524. PMID: 30279368; PMCID: PMC6222472.

[6] Juan Pablo Inostroza, Javiera Troncoso, Claudia Mardones and Carola Vergara Rosales Lignans in olive stones discarded from the oil industry, Comparison of three extraction methods followed by HPLC-DAD-MS/MS and antioxidant capacity determination, June 2018 Journal of the Chilean Chemical Society 63(2):4001-4005 DOI: 10.4067/s0717-97072018000204001

[7] Sanz, C. & Belaj, Angjelina & Tortosa, J.L. & Pérez, A.G. Comparative study of the content of phenolic compounds in olive fruits and leaves for possible use in breeding programs for the functional selection of olive cultivars. Acta Horticulturae. (2020), p.11-18. 10.17660/ActaHortic.2020.1282.3.

[8] Uylaşer, V. & Yildiz, G. The historical development and nutritional importance of olive and olive oil constituted an important part of the Mediterranean diet. *Crit. Rev. Food Sci. Nutr.* 54, p.1092–1101 (2014).

[9] Taiti, Cosimo & Redwan, Mirvat & Marone, Elettra & Atzori, Giulia & Azzarello, Elisa & Mancuso, Stefano. Comparative analysis of Volatile Compounds (potential aromatic ability) in the fruit of 15 olive Italian cultivars. Advances in Horticultural Science. (2018). 32. 10.13128/has-22715.

[10] Artajo, L. S., Romero, M. P., Morelló, J. R. & Motilva, M. J. Enrichment of refined olive oil with phenolic compounds: Evaluation of their antioxidant activity and their effect on the bitter index. *J. Agric. Food Chem.* 54, p.6079–6088 (2006).

[11] Ben-Amor I, Musarra-Pizzo M, Smeriglio A, D'Arrigo M, Pennisi R, Attia H, Gargouri B, Trombetta D, Mandalari G, Sciortino MT. Phytochemical Characterization of *Olea europea* Leaf Extracts and Assessment of Their Anti-Microbial and Anti-HSV-1 Activity. Viruses. 2021 Jun 7;13(6):1085. doi: 10.3390/v13061085. PMID: 34200316; PMCID: PMC8229950.

[12] Pasković I, Lukić I, Žurga P, Majetić Germek V, Brkljača M, Koprivnjak O, Major N, Grozić K, Franić M, Ban D, Marcelić Š, Goreta Ban S. Temporal Variation of Phenolic and Mineral Composition in Olive Leaves Is Cultivar Dependent. Plants (Basel). 2020 Aug 27;9(9):1099. doi: 10.3390/plants9091099. PMID: 32867040; PMCID: PMC7570285.

[13] Olmo-García L, Bajoub A, Benlamaalam S, Hurtado-Fernández E, Bagur-González MG, Chigr M, Mbarki M, Fernández-Gutiérrez A, Carrasco-Pancorbo A. Establishing the Phenolic Composition of *Olea europaea* L. Leaves from Cultivars Grown in Morocco as a Crucial Step Towards Their Subsequent Exploitation. Molecules. 2018 Oct 2;23(10):2524. doi: 10.3390/molecules23102524. PMID: 30279368; PMCID: PMC6222472.

[14] Fu S, Arráez-Roman D, Segura-Carretero A, Menéndez JA, Menéndez-Gutiérrez MP, Micol V, Fernández-Gutiérrez A. Qualitative screening of phenolic compounds in olive leaf extracts by hyphenated liquid chromatography and preliminary evaluation of cytotoxic activity against human breast cancer cells. Anal Bioanal Chem. 2010 May;397(2):643-54. doi: 10.1007/s00216-010-3604-0.

[15] Gergő Tóth, Ágnes Alberti, Anna Sólyomváry, Csenge Barabás, Imre Boldizsár, Béla Noszál, Phenolic profiling of various olive bark-types and leaves: HPLC–ESI/MS study, Industrial

Crops and Products,Volume 67,2015,Pages432-438,ISSN09266690, https://doi.org/10.1016/j.indcrop.2015.01.077.

[16] A. Belaj, M.D. Dominguez-García, S.G. Atienza, N.M. Urdíroz, R. De la Rosa, Z. Satovic, A. Martin, A. Kilian, I. Trujillo, V. Valpuesta, C. Del Rio Developing a core collection of olive (Olea europaea L.) based on molecular markers (DARTs, SSRs, SNPs) and agronomic traits Tree Genet. Genomes, 8 (2012), pp. 365-378, 10.1007/s11295-011-0447-6

[17] Green, 2002 P.S. Green A revision of *Olea* L (*Oleaceae*)Kew Bull., 57 (1) (2002), pp. 91-140, 10.2307/4110824

[18] C.M. Kalua, M.S. Allen, D.R. Bedgood, A.G. Bishop, P.D. Prenzler, K. Robards Olive oil volatile compounds, flavour development and quality: a critical review Food Chem., 100 (1) (2007), pp. 273-286, 10.1016/j.foodchem.2005.09.059

[19] Muzzalupo, I. (Ed.). (2012). Olive Germplasm - The Olive Cultivation, Table Olive and Olive Oil Industry in Italy. InTech. doi: 10.5772/3314

[20] S. Rizwan, C. Benincasa, K. Mehmood, S. Anj um, Z. Mehmood, G. Hussain Alizai, M. Azam, E. Perri, A. Sajjad Fatty acids and phenolic profiles of extravirgin olive oils from selected Italian cultivars introduced in southwestern province of Pakistan J.Oleo Sci., 68 (1) (2019),p. 3343, 10.5650/jos.ess18150

[21] Marra, Roberta & Coppola, Mariangela & Pironti, Angela & Grasso, Filomena & Lombardi, Nadia & D'Errico, Giada & Sicari, Andrea & Censi, Sergio & Woo, Sheridan & Rao, Rosa & Vinale, Francesco. (2020). The Application of Trichoderma Strains or Metabolites Alters the Olive Leaf Metabolome and the Expression of Defense-Related Genes. Journal of Fungi. 6. 369. 10.3390/jof6040369.

[22] Semmar N, Laroussi-Mezghani S, Grati-Kamoun N, Hammami M, Artaud J. A new simplex chemometric approach to identify olive oil blends with potentially high traceability. Food Chem. 2016 Oct 1; 208:150-60. doi 10.1016/j.foodchem.2016.03.087. Epub 2016 Mar 30. PMID: 27132835.

[23] Brenes M, García A, García P, Garrido A. Rapid and complete extraction of phenols from olive oil and determination by means of a coulometric electrode array system. J Agric Food Chem. 2000 Nov;48(11):5178-83. doi: 10.1021/jf000686e. PMID: 11087455.

[24] Sain A, Sahu S, Naskar D. Potential of olive oil and its phenolic compounds as therapeutic intervention against colorectal cancer: a comprehensive review. Br J Nutr. 2022 Oct 14;128(7):1257-1273. doi: 10.1017/S0007114521002919. Epub 2021, Aug 2. PMID: 34338174.

[25] Brenes M, García A, García P, Garrido A. Rapid and complete extraction of phenols from olive oil and determination by means of a coulometric electrode array system. J Agric Food Chem. 2000 Nov;48(11):5178-83. doi: 10.1021/jf000686e. PMID: 11087455.

[26] M.G. Bagur-González, E. Pérez-Castaño, M. Sánchez-Viñas, D. Gázquez-Evangelista, Using the liquid-chromatographic-fingerprint of sterols fraction to discriminate virgin olive from other edible oils,Journal of Chromatography A,Volume 1380,2015,Pages 64-70, https://doi.org/10.1016/j.chroma.2014.12.052.

[27] Amira Allalout, Dhouha Krichène, Kawther Methenni, Ameni Taamalli, Imen Oueslati, Douja Daoud, Mokhtar Zarrouk, Characterization of virgin olive oil from Super Intensive Spanish and Greek varieties grown in northern Tunisia,Scientia Horticulturae,Volume 120, Issue 1,2009,Pages 77-83,ISSN 0304-4238, https://doi.org/10.1016/j.scienta.2008.10.006

[28] Sonda Ammar, Hasim Kelebek, Akram Zribi, Mounir Abichou, Serkan Selli, Mohamed Bouaziz, LC-DAD/ESI-MS/MS characterization of phenolic constituents in Tunisian extra-virgin olive oils: Effect of olive leaves addition on chemical composition, Food Research International, Volume 100, Part 3,2017, Pages 477-485, ISSN: 0963-9969, https://doi.org/10.1016/j.foodres.2016.11.00.

[29] Arumugam Vignesh, Subramaniam Selvakumar, Krishnan Vasanth, Comparative LC-MS analysis of bioactive compounds, antioxidants and antibacterial activity from leaf and callus extracts of Saraca asoca, Phytomedicine Plus, Volume 2, Issue 1,2022,100167, ISSN: 2667-0313, https://doi.org/10.1016/j.phyplu.2021.100167.

[30] Diraman, H.; Dibeklioglu, H. Using lipid profiles for the characterization of Turkish monocultivar olive oils produced by different systems. International Journal of Food Properties 2014, 17, p.1013–1033.

Appendix

Table 1. List of Analyzed Components of Olive Parts

pRT [min]	m/z meas.	M meas.	Name	Molecular Formula	ΔRT	Olive Oil	Olive leaves	Olive Stone	Olive branch	Olive Fruit	Table Olives all
5.59	609.1473	610.1546	Rutin	$C_{27}H_{30}O_{16}$	0.4	0	0	413056	0	0	0
5.86	447.0886	448.0958	Luteolin 7-O-glucoside (Cynaroside)	$C_{21}H_{20}O_{11}$	-0.04	918	1102758	352808	244460	874534	885692
7.22	447.0884	448.0957	Kaempferol-7-O-glucoside	$C_{21}H_{20}O_{11}$	0.23	0	686882	95890	175680	351184	408284
6.03	593.1531	594.1603	3-O-Neohesperidoside Kaempferol (NMR)	$C_{27}H_{30}O_{15}$	0.11	0	0	72792	0	0	0
6.76	447.0884	448.0957	Kaempferol-3-O-glucoside	$C_{21}H_{20}O_{11}$	0.02	0	347812	61376	173824	164896	393188
8.5	285.0395	286.0468	Luteolin	$C_{15}H_{10}O_6$	-0.12	30336	485046	39758	140342	163540	209116
6.55	447.0889	448.0961	Kaempferol-3-O-glucoside	$C_{21}H_{20}O_{11}$	-0.19	0	70356	26778	343538	116456	92738
4.64	609.1464	610.1537	Luteolin-7,3'-di-O-glucoside	C27H30O16	-0.38	0	0	19722	0	0	0
6.77	285.0389	286.0462	3,6,2',4'-Tetrahydroxyflavone	C15H10O6	-0.34	0	73296	16278	46844	46216	86370
2.85	137.0253	138.0326	4-Hydroxybenzoic acid	C7H6O3	0.21	296	0	13236	2536	8628	5584
8.43	301.0332	302.0405	Quercetin	C15H10O7	-0.23	554	179816	13148	303910	13024	132514
1.34	137.0251	138.0324	Protocatechuic aldehyde	C7H6O3	-0.66	0	60028	12826	7026	18098	24510
2.55	137.0255	138.0327	4-Hydroxybenzoic acid	C7H6O3	-0.1	262	3532	9018	10450	6324	3998
1.04	117.0202	118.0274	Succinic acid	C4H6O4	0.05	3488	8394	8754	5228	6852	6688
9.79	269.0447	270.052	Genistein	C15H10O5	-0.14	8942	52560	8548	85054	14092	46202
1.83	153.0195	154.0268	2,5-Dihydroxybenzoic acid	C7H6O4	-0.66	286	24082	6360	8698	11898	10436
0.26	688.702	689.7092				5056	6538	5482	5338	6024	4924
5.28	151.0413	152.0485	2,4-Dihydroxyacetophenone	C8H8O3	-0.4	0	8180	4894	6880	5730	3442
5.7	167.0354	168.0427	5-Methoxysalicylic acid	C8H8O4	-0.36	158	16502	4304	13610	10206	10746
9.4	271.0602	272.0675	naringenin	C15H12O5	-0.24	4762	34490	3974	994948	8114	222410
7.76	151.0406	152.0479	2,6-Dihydroxyacetophenone	C8H8O3	0.85	600	4642	3506	0	2256	3036
4.64	195.0654	196.0727	3,5-Dimethoxy-4-hydroxyacetophenone	C10H12O4	-0.85	0	6632	3164	1446	0	0
2.83	179.0355	180.0428	Caffeic Acid	C9H8O4	-0.47	0	0	3032	2170	1864	2640
3.29	179.0354	180.0427	Caffeic Acid	C9H8O4	-0.01	626	3622	2756	1466	3382	2280
6.5	287.0543	288.0615	Dihydrokaempferol	C15H12O6	-0.03	632	71140	2442	1750180	4258	428770
5.99	121.0307	122.038	Benzoic acid	C7H6O2	0.18	4792	0	2410	598	1684	0
5.7	195.0665	196.0738	3,5-Dimethoxy-4-hydroxyacetophenone	C10H12O4	0.21	1158	4142	2404	5036	2922	0
17.82	487.3445	488.3517	Pygenic acid B a	C30H48O5	-0.38	1200	0	2132	0	0	0
5.3	303.048	304.0558	Taxifolin (3,3',4',5,7-pentahydroxylflavanone)	C15H12O7	0.11	0	172970	2008	420400	8308	116134
5.87	285.0382	286.0455	7,3',4',5'-Tetrahydroxyflavone	C15H10O6	0.57	0	2740	2002	956	2102	2118
1.61	169.0145	170.0218	Gallic Acid	C7H6O5	0.49	0	1428	1942	752	2314	1134
9.96	285.0395	286.0468	Kaempferol	C15H10O6	-0.05	1568	25554	1932	791926	3054	182528

pRT [min]	m/z meas.	M meas.	Name	Molecular Formula	ΔRT	Olive Oil	Olive leaves	Olive Stone	Olive branch	Olive Fruit	Table Olives all
4.4	447.0933	448.1006	ISO-Orientin	C21H20O11	-0.47	0	0	1924	0	0	1478
10.18	299.0545	300.0618	Hispidulin	C16H12O6	-0.33	3524	19304	1766	25010	4206	13976
4.24	609.1488	610.1561	Luteolin-7,3'-di-O-glucoside	C27H30O16	-0.95	374	3432	1630	1258	6310	0
1.84	109.0302	110.0374	Catechol	C6H6O2	-0.66	0	3490	1616	3318	3564	2406
4.5	191.0361	192.0433	Scopoletin	C10H8O4	-0.58	0	2756	1546	408	1246	0
8.53	609.184	610.1912	Neohesperidin	C28H34O15	0.38	0	1968	1518	0	1026	0
7.95	287.0532	288.0605	Eriodictyol	C15H12O6	-0.36	668	59856	1492	104134	2624	39924
21.14	564.3298	565.3371	1-Hydroxy-2-(9Z,12Z,15Z-octadecatrienoyl)-sn-glycero-2-phosphocholine (NMR)	C27H52NO9P	-0.85	98	0	1400	0	0	0
3.19	167.0355	168.0428	Vanillic acid	C8H8O4	-0.09	774	2658	1356	4690	1044	2104
4.4	163.041	164.0483	p-Coumaric acid	C9H8O3	-0.08	700	6486	1274	0	0	3456
28.43	279.2319	280.2391	Pinolenic acid	C18H32O2	-0.73	2224	444	1178	502	876	1026
5.1	193.0505	194.0577	Ferulic acid (trans)	C10H10O4	-0.07	0	2864	1172	2678	0	2280
7.16	151.0409	152.0481	2,6-Dihydroxyacetophenone	C8H8O3	0.25	996	0	1134	0	824	1118
21.45	471.3469	472.3542	Hederagenin	C30H48O4	-0.24	0	19864	1124	4044	5726	5568
29.99	279.2305	280.2378	Linoelaidic acid	C18H32O2	-0.19	1104	0	1072	944	0	584
3.84	167.0363	168.0436	Vanillic acid	C8H8O4	0.56	658	0	1066	1508	2728	160
4.84	463.0925	464.0998	Hyperoside	C21H20O12	-0.79	0	23336	1004	0	0	0
6.81	151.0402	152.0475	2,6-Dihydroxyacetophenone	C8H8O3	-0.1	658	0	838	1292	558	1028
26.45	297.2442	298.2515	(Z)-3-Hydroxyoctadec-7-enoic acid (NMR)	C18H34O3	-0.48	902	586	786	674	834	616
2.69	109.0306	110.0379	Catechol	C6H6O2	0.19	0	1372	718	468	1254	616
7.81	359.0725	360.0797	Rosmarinic acid	C18H16O8	0.9	0	5570	712	1074	296	438
2.37	167.0342	168.0415	Vanillic acid	C8H8O4	-0.91	0	2420	700	1878	630	0
3.57	287.0545	288.0617	3,7,3',4'-Tetrahydroxyflavanone (Fustian)	C15H12O6	-0.93	0	4566	614	159218	482	28140
26.74	297.2429	298.2502	(Z)-3-Hydroxyoctadec-7-enoic acid (NMR)	C18H34O3	-0.19	954	530	578	798	474	1074
26.57	297.2422	298.2495	(Z)-3-Hydroxyoctadec-7-enoic acid (NMR)	C18H34O3	-0.36	912	792	572	348	1094	734
26.14	297.2415	298.2488	(Z)-3-Hydroxyoctadec-7-enoic acid (NMR)	C18H34O3	-0.79	0	704	548	0	288	1012
7.65	285.0385	286.0458	3,6,3',4'-Tetrahydroxyflavone	C15H10O6	0.17	0	0	340	1078	1474	524
12.38	285.0368	286.0441	7-Hydroxy-2'-methoxyflavone	C15H10O6	0.49	210	4772	302	1838	416	1920
6.73	301.0326	302.0399	Tricetin	C15H10O7	-0.87	0	7306	298	24184	2654	8560
29.42	279.2284	280.2357	10E, 12Z-Linoleic acid	C18H32O2	-0.16	0	1132	296	562	862	868
6.2	285.0377	286.045	7,3',4',5'-Tetrahydroxyflavone	C15H10O6	-0.91	0	488	284	936	244	484
3.64	353.0828	354.0901	Chlorogenic acid	C16H18O9	0.68	0	2822	256	1122	0	876

pRT [min]	m/z meas.	M meas.	Name	Molecular Formula	ΔRT	Olive Oil	Olive leaves	Olive Stone	Olive branch	Olive Fruit	Table Olives all
11.27	315.048	316.0553	ISOHAMNETIN	C16H12O7	0.84	0	904	240	716	0	272
7.92	147.0468	148.0541	Cinnamic Acid	C9H8O2	-0.74	1086	374	236	506	266	406
3.62	179.0354	180.0427	Caffeic Acid	C9H8O4	0.31	0	1310	226	1068	824	350
4.13	179.0344	180.0416	Caffeic Acid	C9H8O4	0.82	0	1544	204	406	410	416
7.27	301.032	302.0392	Tricetin	C15H10O7	-0.33	0	764	184	3016	0	924
10.34	315.0471	316.0544	ISOHAMNETIN	C16H12O7	-0.1	0	60990	178	59876	548	38540
3.77	289.07	290.0773	Epicatechin	C15H14O6	0.15	0	0	160	220	25146	5584
9.4	301.031	302.0383	Quercetin	C15H10O7	0.74	0	1322	142	2762	254	1066
5.36	121.0305	122.0378	Benzoic acid	C7H6O2	-0.45	0	0	0	1000	320	0
6.45	137.0246	138.0318	Salicylic acid	C7H6O3	0.8	0	0	0	286	0	1020
5.62	137.0249	138.0322	Salicylic acid	C7H6O3	-0.03	1612	1430	0	556	532	0
5.58	151.0406	152.0479	2,4-Dihydroxyacetophenone	C8H8O3	-0.1	916	27582	0	7966	0	11878
4.52	151.0409	152.0482	Vanillin	C8H8O3	0.28	1640	17032	0	29236	188	11666
2.57	153.0195	154.0268	2,5-Dihydroxybenzoic acid	C7H6O4	0.08	0	1060	0	822	2214	604
4.64	161.025	162.0323	Umbelliferone	C9H6O3	0	0	0	0	2952	0	596
4.06	163.0407	164.048	p-Coumaric acid	C9H8O3	-0.43	0	3576	0	1402	0	0
4.74	163.041	164.0483	p-Coumaric acid	C9H8O3	0.25	106	3220	0	956	0	0
4.1	167.0349	168.0422	Vanillic acid	C8H8O4	0.82	0	1120	0	0	0	178
6.59	177.0194	178.0267	Aesculetin	C9H6O4	-0.32	0	330	0	1550	0	264
2.48	179.0353	180.0426	Caffeic Acid	C9H8O4	-0.83	0	0	0	4038	2196	1360
6.12	195.0677	196.075	3,5-Dimethoxy-4-hydroxyacetophenone	C10H12O4	0.63	1590	0	0	0	0	0
29.93	255.2314	256.2387	Palmitic acid (NMR)	C16H32O2	-0.73	0	0	0	1392	1078	0
28.17	279.2311	280.2384	Pinolenic acid	C18H32O2	-0.99	0	612	0	810	1144	1056
10.98	285.0368	286.0441	7-Hydroxy-2'-methoxyflavone	C15H10O6	-0.91	0	3216	0	0	1356	0
10.78	285.0379	286.0451	Kaempferol	C15H10O6	0.77	0	0	0	7122	982	0
6.13	287.0535	288.0608	Dihydrokaempferol	C15H12O6	-0.4	0	0	0	1076	142	0
13.19	299.0517	300.059	Kaempferide	C16H12O6	-0.82	0	0	0	2018	0	308
7.71	301.032	302.0393	Morin	C15H10O7	0.11	0	472	0	532	5736	3420
5.21	301.0324	302.0397	3,7,3',4',5'-Pentahydroxyflavone (Robinetin)	C15H10O7	-0.14	0	522	0	9696	436	2154
5.78	301.0328	302.04	3,7,3',4',5'-Pentahydroxyflavone (Robinetin)	C15H10O7	0.43	0	98	0	1662	364	864
4.28	303.0496	304.0569	Taxifolin (3,3',4',5,7-pentahydroxylflavanone)	C15H12O7	-0.91	0	548	0	1232	3226	808
6.46	359.0728	360.0801	Rosmarinic acid	C18H16O8	-0.45	0	1020	0	0	0	326
5.36	433.1096	434.1169	3-Glu-3,4',7-trihydroxyisoflavanone (NMR)	C21H22O10	0.9	0	0	0	1756	3164	806
28.34	455.3485	456.3558	Ursolic acid	C30H48O3	0.81	0	0	0	754	368	1052
20.92	471.3504	472.3577	Hederagenin	C30H48O4	-0.77	1186	0	0	0	0	0

Contribution of Individual Authors to the Creation of a Scientific Article (Ghostwriting Policy)

The authors equally contributed to the present research, at all stages from the formulation of the problem to the final findings and solution.

Sources of Funding for Research Presented in a Scientific Article or Scientific Article Itself

The authors acknowledge Applied Science Private University, Amman, Jordan, for the full financial support granted to this research article. Sincere thanks to all my Colleagues in the basic science department, for creating inspiring conditions for work.

Conflict of Interest

The authors have no conflict of interest to declare.