TAXONOMICAL IMPLICATIONS OF NATURAL COMPONENTS IN DELIMITATION OF SOME SPECIES OF ASTERACEAE FAMILY IN BAGHDAD

Rasha A. Al- Souz — Researcher
H. R. H. Al-Newani — Assist. Prof.
Dept. Bio-Coll. Sci., Mustansiriyah University
Email: sphh@uomustansiriyah.edu.iq

ABSTRACT

This study aimed to investigate the taxonomical relationship among eight species belonging to Asteraceae based on natural products as fresh leaves of eight species (*Carthamus tinctorius* L., *Centaurea iberica* Trevir. ex Spreng., *Conyza bonariensis* (L.) Cronquist, *Conyza canadensis* (L.) Cronquist, *Launaea mucronata* (Forssk.) Muschl., *Senecio glaucus* L., *Sonchus asper* (L.) Hill, and *Sonchus tenerrimus* L.) have been collected from different regions of Baghdad. The phytochemical screening of hexane extracts from eight plants showed different secondary metabolites in the studied species. Gas chromatography-mass spectrometry (GC-MS) analysis of eight hexane extracts showed the existence of eighty-one chemical compounds of eight taxa of Asteraceae, including hydrocarbons, alcohols, organic acids, esters, amines, and heterocyclic compounds. The agglomerative hierarchical clustering analysis dendrogram was carried out depending on 81 chemical compounds of the eight taxa of Asteraceae, gained by Euclidean distance using Ward's method. The HCA dendrogram showed the closeness of *Sonchus asper* and *Sonchus tenerrimus* and a divergence between *Conyza canadensis* and *Conyza bonariensis* and their affinity to *Launaea mucronata* while *Carthamus tinctorius* is the most divergent species from the rest of the species.

Keywords: **Secondary metabolites, phytochemical analysis, Compositae family, HCA dendrogram.**

الاهمية التصنيفية للمركبات الطبيعية في عزل و تصنيف بعض اجناس العائلة المركبة في بغداد

رشا عبد الرحيم السوز — **باحث**
هديل رضاوي حسين النويني — **استاذ مساعد**
قسم علوم الحياة ,كلية العلوم , الجامعة المستنصرية

المستخلص:

هذه الدراسة تهدف الى التحري عن العلاقات التصنيفية بين ثمانية انواع تعود الى العائلة المركبة على اساس المركبات الطبيعية حيث تم جمع اوراق يانعة لثمانية أنواع (*Carthamus tinctorius* L., *Centaurea iberica* Trevir. ex Spreng., *Conyza bonariensis* (L.) Cronquist, *Conyza canadensis* (L.) Cronquist, *Launaea mucronata* (Forssk.) Muschl., *Senecio glaucus* L., *Sonchus asper* (L.) Hill, and *Sonchus tenerrimus* L.) من مناطق مختلفة من بغداد.أظهر الفحص الكيميائي النباتي لمستخلصات الهكسان لثمانية نباتات وجود اختلافات في المركبات الثانوية في الأنواع المدروسة. أظهر تحليل كروماتوغرافيا لمستخلصات الهكسان وجود واحد وثمانين مركبًا كيميائيًا لثمانية أصناف من العائلة المركبة، بما في ذلك الهيدروكربونات والكحوليات والأحماض العضوية والإسترات والأمينات والمركبات الحلقية غير المتجانسة. تم إجراء تحليل هرمي للتحليل التجميعي العنقودي اعتمادًا على 81 مركبًا كيميائيًا من الانواع الثمانية لنباتات العائلة المركبة، تم اعتماده عن طريق المسافة الإقليدية باستخدام طريقة وارد.أظهر المخطط الشجري HCA تقارب *Sonchus asper* و *Sonchus tenerrimus* و الاختلاف بين *Conyza canadensis* و *Conyza bonariensis* وتقاربهما مع *Launaea mucronata* في حين أن *Carthamus tinctorius* هو أكثر الأنواع اختلافًا عن بقية الأنواع.الكلمات المفتاحية : مركبات الايض الثانوي، التحليل الكيميائي النباتي، العائلة المركبة، المخطط الشجري لتحليل التجميع الهرمي.

الكلمات المفتاحية : مركبات الايض الثانوي، التحليل الكيميائي النباتي، العائلة المركبة، المخطط الشجري لتحليل التجميع الهرمي.

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INTRODUCTION

Nowadays, the application of secondary metabolites as chemical markers in chemotaxonomy has been used widely by taxonomists and botanists, as many studies demonstrated the role of natural compounds in solving the taxonomic problems. The occurrence of isolated natural substances has also been employed to illustrate similarities among different plant groups (40). The Asteraceae family, commonly known as the daisy family, is one of the largest and most diverse plant families in the world, with more than 23,000 species distributed worldwide. This family is characterized by its great morphological diversity, including herbaceous, shrubby, and climbing species, and its habitats range from desert to humid regions (31.33).

In Iraq, Asteraceae family represents an important component of the vegetation, contributing to the formation of various ecosystems and playing a vital role in maintaining biodiversity (17). Baghdad City witnessed major environmental changes due to the wars and conflicts that the country experienced, which affected the plant diversity in the region (3,7). This has led to a change in the distribution and abundance of some Asteraceae species and perhaps to a change in their ability to adapt and photosynthesize in their new environments (6, 19,20,38).

This study aims to explore the chemical diversity of some Asteraceae species in Baghdad. Using hierarchical clustering analysis (HCA) as a multivariate statistical tool to explore the relationships between different species based on their chemical composition (5, 9).

MATERIALS AND METHODS

Plants collections

Fresh leaves of eight species were collected during the summer season of 2023 from different regions of Baghdad. The specimens have been identified by the curator of Mustansiriyah University Herbarium; however, the plant scientific names were checked at https://powo.science.kew.org/, and then the samples were rinsed with water and dried in air for two weeks at 25 °C and preserved in the herbarium.

Plant extracts and phytochemicals analysis

Twenty grams of dried plant material were extracted with 100 ml of hexane for 6 hours at room temperature. The extracts were filtered and stored at 4°C (2). Phytochemical analysis was performed using the colorimetric method by using tests illustrated by (18,25,36). The phytochemical analysis was examined at the Ibn al-Baytar Research Center - Iraqi Ministry of Industry and Minerals Corporation of Research and Industrial Development**.**

Plant extracts and GC/MS analysis

Dried leaves of eight species from Asteraceae family were extracted using an ultrasonic probe (Q700CA Sonicator, USA) with n-hexane (1:20 g/ml solvent/sample ratio) for 15 min at 20 kHz. The extract was filtered and stored at 4 °C (26). Gas chromatography–mass spectrometry (GC/MS) analysis was performed on an Agilent 7820A with a HP-5 ms column (30 m × 250 μm) using helium as the carrier gas. The inlet and injector temperatures were 250 °C. The injection volume was 1 μl in splitless mode. Mass spectra were acquired at a rate of 10,000 units/s over a mass range of 25 to 1000 m/z. Compound identification was based on retention time (1). The chemical classification of chemical compounds produced by GC/MS was based on (10, 24).

HCA Dendrogram Analysis

A hierarchical cluster analysis using Ward's method and Euclidean distance was performed on 81 chemical compounds from eight species of the Asteraceae family to determine their relationships. The analysis was performed using SPSS version 26.0. (11,28).

RESULTS AND DISCUSSION

Phytochemicals screening

Chemical analysis of non-polar crude hexane extracts from eight species showed that the most prevalent phytochemicals were glycosides and carbohydrates in all taxa. Flavonoids were found in all taxa except *Launaea mucronata*, while resins were recorded in all taxa except *Senecio glaucus*. Tannins and terpenes were observed in five taxa, while tannins were not recorded in three taxa (*Carthamus tinctorius*, *Conyza bonariensis, and Senecio glaucus*) and terpenes were absent in (*Centaurea iberica*, *Conyza bonariensis*, *and Sonchus asper*). Coumarins were found in *Conyza canadensis*, *Launaea mucronata*, and *Senecio glaucus*.

However, alkaloids were documented only in two taxa, *Senecio glaucus* and *Sonchus tenerrimus*. Phenols, proteins, saponins, and steroids were not detected in any studied taxa., as illustrated in Table 1.

The current results agreed with (8) as they reported the phytoconstituents of some of these plants**.** However, different phytochemical compounds were identified in some plant species, suggesting that phytochemical composition can vary depending on various factors such as geographical location, environmental conditions, and plant age (12).

Table 1. Phytochemicals analysis of hexane extracts of studied species

Species / Phytochemicals tests	*Carthamus tinctorius*	*Centaurea iberica*	*Conyza bonariensis*	*Conyza canadensis*	*Launaea mucronata*	*Senecio glaucus*	*Sonchus asper*	*Sonchus tenerrimus*
Alkaloids Test	-	-	-	-	-	+	-	+
Glycosides Test	+	+	+	+	+	+	+	+
Phenols Test	-	-	-	-	-	-	-	-
Flavonoids Test	+	+	+	+	-	+	+	+
Tannins Test	-	+	-	+	+	-	+	+
Coumarins Test	-	-	-	+	+	+	-	-
Terpenes Test	+	-	-	+	+	+	-	+
Resins Test	+	+	+	+	+	-	+	+
Protein Test	-	-	-	-	-	-	-	-
Carbohydrate Test	+	+	+	+	+	+	+	+
Saponin Test	-	-	-	-	-	-	-	-
Steroids Test	-	-	-	-	-	-	-	-

Gas chromatography-mass spectrometry (GC-MS) analysis

Gas chromatography-mass spectrometry (GC-MS) analysis of eight hexane extracts showed the existence of eighty-one chemical compounds of eight taxa of Asteraceae, including hydrocarbons, alcohols, organic acids, esters, amines, and heterocyclic compounds as listed in Tables from 2 to 9. *Centaurea iberica* had the highest chemical diversity with 29 compounds, followed by *Conyza bonariensis* and *Launaea mucronata* with 17 each. *Conyza canadensis* produced 12 compounds, *Sonchus asper* 11, *Senecio glaucus* 10, and *Sonchus tenerrimus* had the fewest with 6 compounds.The most common compounds that have been identified are Octadecanoic acid, Hexadecanoic acid, methyl ester, 9-Octadecenoic acid (Z)-, methyl ester, Eicosane, and 2-Heptadecanone. However, the chemical compounds that were abundant across species were 3-Hexanone, 2,5-cyclohexadien-1-one,2,6-bis (1,1-dimethylethyl)-4-methylene-, Tetracosane, Nonadecane, Eicosane, Eicosyl isopropyl ether, Nonane (Volatile oil) and 2-Heptadecanone.In addition, several unique compounds were detected in each species, such as1H-Imidazo[1,2-a] imidazole, 2-(4-methoxyphenyl)-1,5,6-triphenyl- in *Carthamus tinctorius*, and Fagaronine and 14-.Beta.-H-Pregna in *Centaurea iberica*, 18-Pentatriacontanone in *Conyza bonariensis*,(22-Z)-Dehygrocholesterol-1-Ether,Tetrahydrofuran-2-carboxylic acid,dibenzofuran-3-ylamide and p-Camphorene in *Conyza canadensis*, Nonacosane in *Launaea mucronata*, Nonyl Docosanoate in *Senecio glaucus*, Ethanone, 1,1'-[3,3'-biisoxazole]-5,5'-diylbis- in *Sonchus asper*, and Stigmasterol in *Sonchus tenerrimus.*The previous results agreed with (37, 39, 41) as they reported that Asteraceae species are rich in fatty acids such as Octadecanoic acid and Hexadecanoic acid (Palmitic acid). The main hydrocarbon compounds were Nonacosane, Tricosane, and Cyclotetracosane. The major representative alcohols were 2-Octadecyloxy-1,1,2,2-Tetradeuteroethanol and 2-Tetradecanol (myristyl alcohol). Main oxygen-containing compounds (20R)-6-Aza-7-oxo-5.alpha.-pregnan-3.beta.,20-diyl acetate benzoate , 3',7'-Dimethyloct-6'-enyl 3-methyl-2-oxopentadecanoate and 2-Heptadecanone. Stigmasterol is an unsaturated phytosterol. The main aromatic compounds were 2,5-cyclohexadien -1- one, 2, 6- bis (1,1-dimethylethyl) -4- methylene- and 1, 2-Benzenedicarboxylic acid,bis(2-ethylhexyl) ester. Numerous additional valuable chemical compounds were detected in this study, such as Heptadecane, a critical element in essential oil production and shown to possess both anti-inflammatory and antimicrobial effects (34). 14-. Beta. -H-Pregna is a naturally occurring compound derived from steroid hormones and acts as an adrenergic receptor with antimicrobial and anti-inflammatory benefits (10). The study showed that the species *Centaurea iberica* contains the compound Fagaronine, which is a benzo phenanthrene alkaloid considered as a mutagen (30). Moreover, the species contained 9-Octadecenoic acid(Z)-,9-hexadecenyl ester, (Z)-. Numerous studies have demonstrated that octadecanoic fatty acid effectively inhibits the growth of *Pseudomonas aeruginosa* (15). *Conyza bonariensis* exhibited the presence of DL-Glutamic-2-d acid, N-acetyl-, dimethyl ester ($C_9H_{14}2DNO_5$) that contains Deuterium (D), which is a stable isotope of hydrogen, also known as heavy hydrogen (D^2), Deuterium has a significant effect on biological systems, various morphological changes have been observed in cells and organisms treated with deuterium. Deuteration alters or disrupts many physiological processes, disrupting the cell cycle by blocking cell division and preventing DNA replication (22). *Conyza bonariensis* also contain the compound 2-(4'-Nitrophenyl) quinoxaline-1,4-dioxide, which is one of the Quinoxaline derivatives and they are used against bacteria, fungi, conditions of viral infections, leishmaniasis, TB, malaria and cancer (21). The results showed that *Launaea mucronata* contains 2-Tetradecanol compound could result in immunosuppressive effects on disorders mediated by T cells (29). On the other hand, *Sonchus asper* contains important chemical compounds 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester, as this compound has antibacterial activity (14). In addition, *Conyza canadensis* contains several significant compounds including a highly toxic and carcinogenic Di-(2-ethylhexyl) phthalate compound (DEHP), which is not produced naturally in plants, and its presence may reflect environmental pollution and the role of this plant in phytoremediation; this compound is widely used as a plasticizer in many industries (32). Tetrahydrofuran-2-carboxylic acid, dibenzofuran-3-ylamide is also a significant component found in *Conyza canadensis*; it is a volatile organic molecule utilized in cancer chemotherapy (4). However, diverse chemical compounds were found in this research, indicating that the plants' composition can change depending on various factors such as harvest season, plant age, and environment (13,16).

Table 2. GC-MS of the species *Carthamus tinctorius*

Peak No.	Chemical compounds	Retention Time (min.)	Area% 100%	Molecular formula	Molecular weight (g/mol)	Chemical classification
1	3-Hexanone	7.734	1.21	$C_6H_{12}O$	100.16	Ketone
2	2,5-cyclohexadien-1-one,2,6-bis(1,1-dimethylethyl)-4-methylene-	38.150	5.49	$C_{15}H_{22}O$	218.33	Unsaturated cyclic ketone
3	Nonadecane	53.999	1.21	$C_{19}H_{40}$	268.5	Alkane
4	trans-13-Octadecenoic acid, methylester	60.389	1.63	$C_{19}H_{36}O_2$	296.48	Unsaturated fatty acid methyl ester
5	Fumaric acid, 2-decyl tridecyl ester	62.578	3.43	$C_{27}H_{50}O_4$	438.68	Diester of fumaric acid
6	Decanedioic acid, bis(1,2,2,6,6-pentamethyl-4-piperidinyl) ester	64.161	50.26	$C_{30}H_{56}N_2O_4$	508.8	Diester derived from decanedioic acid
7	6-Hexadecenoic acid, 7-methyl, methyl ester E	66.030	6.69	$C_{18}H_{34}O_2$	282.5	Unsaturated fatty acid
8	1H-Imidazo[1,2-a]imidazole,2-(4-methoxyphenyl)-1,5,6-triphenyl-	67.481	25.78	$C_{30}H_{23}N_3O$	441.53	Heterocyclic organic compound
9	1-Propanone,3-(2-hydroxyphenyl)-1,3-diphenyl-	68.813	2.08	$C_{21}H_{18}O_2$	302.37	Aromatic ketone
10	Heneicosane, 3-methyl-	69.367	2.22	$C_{22}H_{46}$	310.6	Branched alkane

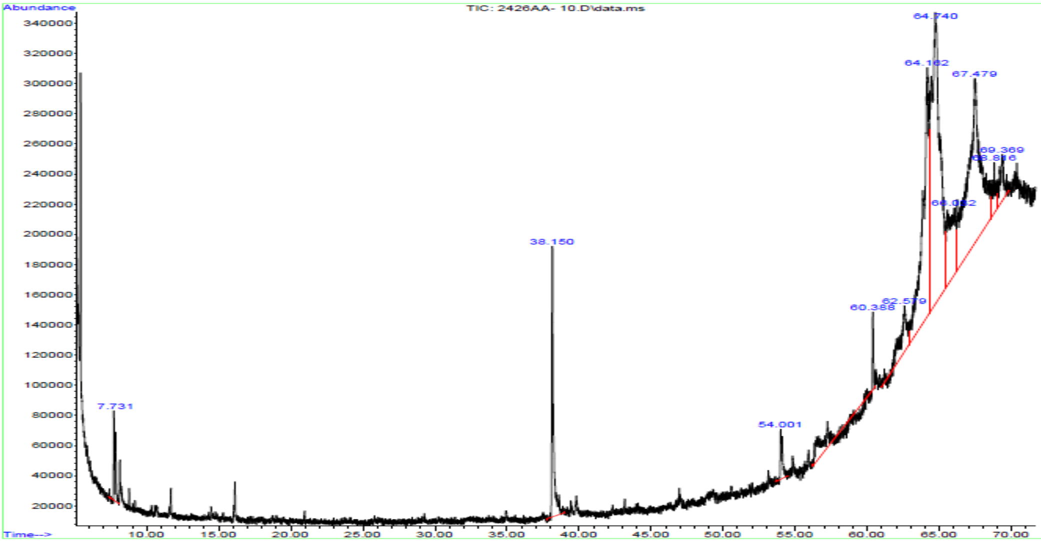

Figure 1. The chromatogram of the GC-MS analysis of the species *Carthamus tinctorius*

Table 3. GC-MS of the species *Centaurea iberica*

PEAK NO.	CHEMICAL COMPOUNDS	RETENTION TIME (MIN.)	AREA% 100%	MOLECULAR FORMULA	MOLECULAR WEIGHT (G/MOL)	CHEMICAL CLASSIFICATION
1	3-Hexanone	7.734	0.26	$C_6H_{12}O$	100.16	Ketone
2	Hexane,2,4-DimethylI-	8.151	0.16	C_8H_{18}	114.23	Branched alkane
3	2,5-cyclohexadien-1-one,2,6-bis (1 ,1-dimethylethyl)-4-methylene-	38.150	1.22	$C_{15}H_{22}O$	218.33	Unsaturated cyclic ketone
4	Heptadecane	46.952	0.23	$C_{17}H_{36}$	240.47	Alkane
5	Cyclotetradecane	48.215	0.67	$C_{14}H_{28}$	196.37	Cycloalkane
6	Octadecane	50.553	0.48	$C_{18}H_{38}$	254.49	Alkane
7	Cyclotetracosane	51.147	1.49	$C_{24}H_{48}$	336.64	Cycloalkane
8	Tetracosane	52.319	4.85	$C_{24}H_{50}$	338.66	Alkane
9	Z-5-Nonadecene	53.136	0.64	$C_{19}H_{38}$	266.5	Alkene
10	Nonadecane	53.982	4.7	$C_{19}H_{40}$	268.5	Alkane
11	1,19-Eicosadiene	55.696	1.19	$C_{20}H_{38}$	278.5	Alkadiene or diene
12	Iron, tricarbonyl [(2,3,4, 5-.eta.)-2,3,4,5-tetrahydroxy-2,4-cyclopentadien-1-one]-	56.439	0.84	$C_8H_4FeO_8$	283.957	Organometallic compound
13	Eicosane	57.251	0.43	$C_{20}H_{42}$	282.5	Alkane
14	Docosane	58.634	0.68	$C_{22}H_{46}$	310.6006	Alkane
15	Oxalic acid,hexadecyl 2-phenylethyl ester	59.074	1.25	$C_{26}H_{42}O_4$	418.6	Diester
16	Heneicosane	60.377	2.35	$C_{21}H_{44}$	296.6	Alkane
17	9-Tricosene, (Z)-	60.829	2.38	$C_{23}H_{46}$	322.6	Alkene
18	Pentacosane	61.492	21.55	$C_{25}H_{52}$	352.7	Alkane
19	Citronellyl palmitoleate	61.886	1.88	$C_{25}H_{52}$	352.68	Ester
20	Heptacos-1-ene	62.503	2.05	$C_{27}H_{54}$	378.71	Alkene
21	Bis(2-ethylhexyl) phthalate	63.241	23.5	$C_{24}H_{38}O_4$	390.56	Diester
22	Succinic acid,3,7-dimethyloct-6-en-1-yl octyl ester	63.869	4.29	$C_{22}H_{40}O_4$	368.55	Ester
23	14-. Beta. -H-Pregna	65.121	0.62	$C_{21}H_{36}$	288.5	Steroid
24	cis-15-Tetracosenoic acid,propyl ester	65.853	0.41	$C_{27}H_{52}O_2$	408.7	Ester of unsaturated fatty acid
25	Dodecane, 1-(methoxymethoxy)-	66.984	2.76	$C_{14}H_{30}O_2$	230.39	Ether
26	Fagaronine	67.744	8.77	$C_{21}H_{20}NO_4$	350.39	Benzophenanthridine alkaloid
27	3-(1,3-Diphenyl-1H-pyrazol-5-yl)-1-methyl-1H-indole	68.379	3.46	$C_{24}H_{19}N_3$	349.4	Heterocyclic organic compound
28	9-Octadecenoic acid(Z)-,9-hexadecenyl ester, (Z)-	68.996	1.72	$C_{34}H_{64}O_2$	504.9	Ester
29	3-Butyl-2-(acrydin-9'-yl) imino-1,3-thiazolidin-2-one	69.705	5.17	$C_{20}H_{19}N_3OS$	349.45	Heterocyclic organic compound

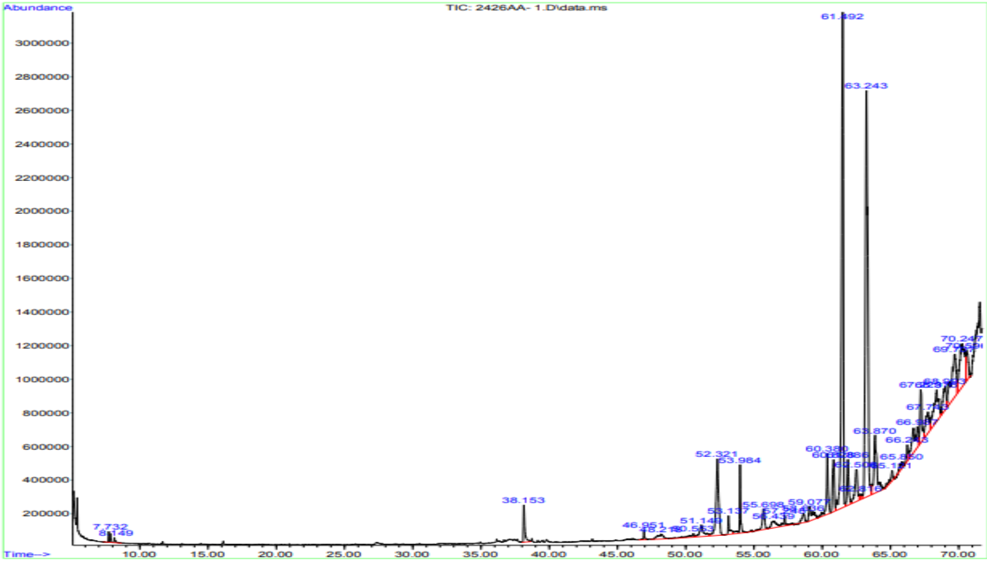

Figure 2. The chromatogram of the GC-MS analysis of the species *Centaurea iberica*

Table 4. GC-MS of the species *Conyza bonariensis*

Peak No.	Chemical compounds	Retention Time (min.)	Area% 100%	Molecular formula	Molecular weight (g/mol)	Chemical classification
1	3-Hexanone	7.734	0.28	$C_6H_{12}O$	100.16	Ketone
2	DL-Glutamic-2-d acid,N-acetyl-,dimethyl ester	8.151	0.15	$C_9H_{14}2DNO_5$	218.23	Modified amino acid diester
3	2,5-cyclohexadien-1-one,2,6-bis (1 ,1-dimethylethyl)-4-methylene-	38.156	1.59	$C_{15}H_{22}O$	218.33	Unsaturated cyclic ketone
4	Tricosane	53.999	0.2	$C_{23}H_{48}$	324.6	Alkane
5	Succinic acid,2,5-difluorobenzylheptadecyl ester	54.833	0.5	$C_{28}H_{44}F_2O_4$	482.64	Ester
6	Ethanone,1-(2-thiazolyl)-	57.251	3.15	C_5H_5NOS	127.17	Heterocyclic ketone
7	S-Chloro-S-fluoro-N-pentafluorosulfanylsulfilimine	58.543	2.4	ClF_6NS_2	227.6	Sulfilimine or (sulfimide)
8	N-[2-(2-isopropylphenoxy)ethyl]naphthalene-2-sulfonamid	59.428	4.15	$C_{21}H_{23}NO_3S$	369.48	Sulfonamide
9	4-Hexen-3-one, O-methyloxime	59.754	13.54	$C_7H_{13}NO$	127.18	Unsaturated ketone
10	(20R)-6-Aza-7-oxo-5. alpha. -pregnan-3. beta.,20-diyl acetate benzoate	60.377	4.64	$C_{29}H_{39}NO_5$	481.6	Modified steroid
11	1-(2'-Acetoxyethoxymethyl)-5-(2,4-difluorobenzylamino) uracil	61.972	7.56	$C_{16}H_{17}F2N_3O_5$	369.32	pyrimidine derivatives
12	Tetracosane	64.378	4.63	$C_{24}H_{50}$	338.7	Alkane
13	3',7'-Dimethyloct-6'-enyl 3-methyl-2-oxopentadecanoate	65.430	1.24	$C_{26}H_{48}O_3$	408.7	Ester
14	18-Pentatriacontanone	67.550	8.85	$C_{35}H_{70}O$	506.9	Ketone
15	4H-1-Benzothiopyran-4-one,3-[(4-methylphenyl) amino]-,1-oxide	67.933	23.95	$C_{16}H_{13}NO_3S$	299.34	Heterocyclic organic compound
16	Octadecanoic acid,ethenyl ester	69.179	11.28	$C_{20}H_{38}O_2$	310.51	Ester
17	2-(4'-Nitrophenyl) quinoxaline-1,4-dioxide	70.368	11.89	$C_{14}H_9N_3O_4$	283.24	Heterocyclic compound

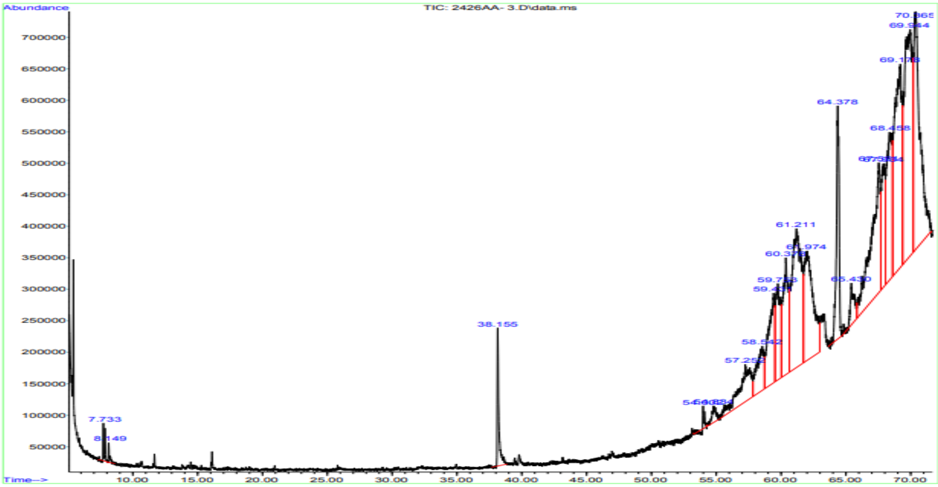

Figure 3. The chromatogram of the GC-MS analysis of the species *Conyza bonariensis*

Table 5. GC-MS of the species *Conyza canadensis*

PEAK NO.	CHEMICAL COMPOUNDS	RETENTION TIME (MIN.)	AREA% 100%	MOLECULAR FORMULA	MOLECULAR WEIGHT (G/MOL)	CHEMICAL CLASSIFICATION
1	3-Hexanone	7.728	1.96	$C_6H_{12}O$	100.16	Ketone
2	Oxirane, 2-ethyl-3-propyl-, cis-	8.145	1.33	$C_7H_{14}O$	114.19	Organoheterocyclic compounds
3	Nonane	11.671	0.82	C_9H_{20}	128.25	Alkane
4	(1R)-2,6,6-Trimethylbicyclo [3.1.1] hept-2-ene	13.266	1.16	$C_{10}H_{16}$	136.234	Alkene
5	2,5-cyclohexadien-1-one,2,6-bis (1 ,1-dimethylethyl)-4-methylene-	38.150	15.65	$C_{15}H_{22}O$	218.33	Unsaturated cyclic ketone
6	2-Heptadecanone	54.096	3.07	$C_{17}H_{34}O$	254.45	Ketone
7	p-Camphorene	56.840	3.42	$C_{20}H_{32}$	272.468	Terpens
8	Docosanoic acid, docosyl ester	59.983	0.1	$C_{44}H_{88}O_2$	649.168	Carboxylic acid
9	Eicosyl isopropyl ether	60.372	0.81	$C_{23}H_{48}O$	340.6	Ether
10	Di-(2-ethylhexyl) phthalate	63.161	15.03	$C_{24}H_{38}O_4$	390.6	Aldehyde or diester of phthalic acid
11	(22-z)-dehydrocholesterol-1-ether	67.344	29.26	$C_{28}H_{46}O$	398.7	Ether
12	Tetrahydrofuran-2-carboxylic acid, dibenzofuran-3-ylamide	71.419	27.39	$C_{17}H_{15}NO_3$	281.3	Amide

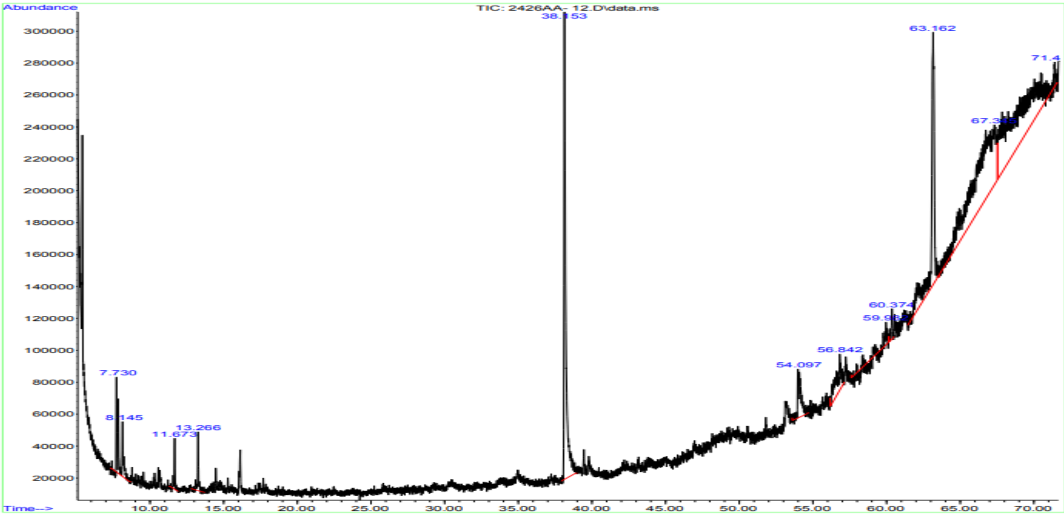

Figure 4. The chromatogram of the GC-MS analysis of the species *Conyza canadensis*

Table 6. GC-MS of the species *Launaea mucronata*

PEAK NO.	CHEMICAL COMPOUNDS	RETENTION TIME (MIN.)	AREA % 100%	MOLECULAR FORMULA	MOLECULAR WEIGHT (G/MOL)	CHEMICAL CLASSIFICATION
1	3-Hexanone	7.734	1.93	$C_6H_{12}O$	100.16	Ketone
2	1,1-Difluorooctane	8.151	1.15	$C_8H_{16}F_2$	150.21	Haloalkane or alkyl halide compound
3	Nonane	11.671	0.9	C_9H_{20}	128.25	Alkane
4	Decane	16.112	1.37	$C_{10}H_{22}$	142.28	Alkane
5	2,5-cyclohexadien-1-one,2,6-bis (1 ,1-dimethylethyl)-4-methylene-	38.156	4.4	$C_{15}H_{22}O$	218.33	Unsaturated cyclic ketone
6	2-Heptadecanone	54.073	2.02	$C_{17}H_{34}O$	254.5	Ketone
7	Hexadecanoic acid,methyl ester	54.828	2.21	$C_{17}H_{34}O_2$	270.5	Ester
8	Hexadecanoic acid ,2-(octadecyloxy)ethyl ester	57.245	2.69	$C_{36}H_{72}O_3$	553	Ester
9	Decane,3,8-dimethyl-	60.383	1.31	$C_{12}H_{26}$	170.33	Alkane
10	2-Tetradecanol	60.577	0.62	$C_{14}H_{30}O$	214.39	Alcohol
11	Eicosyl isopropyl ether	63.366	9.33	$C_{23}H_{48}O$	340.6	Ether
12	cis-3,3a,4,5,6,7-Hexahydro-7-(2-thienyl) cyclohexa[c]isoxazole	64.829	5.6	$C_{11}H_{13}NOS$	207.29	Heterocyclic compound
13	Nonacosane	66.235	33.19	$C_{29}H_{60}$	408.8	Alkane
14	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3. alpha.,5a. alpha9.alpha.,9a. alpha.)]-	67.801	8.03	$C_{15}H_{26}O$	222.366	Cyclic ether
15	Fumaric acid,4-cyanophenyl dodecyl ester	68.327	3.88	$C_{23}H_{31}NO_4$	385.5	Ester
16	Tetracosane	69.190	12.97	$C_{24}H_{50}$	338.7	Alkane
17	i-Propyl 9-octadecenoate	70.116	8.4	$C_{21}H_{40}O_2$	324.54	Ester

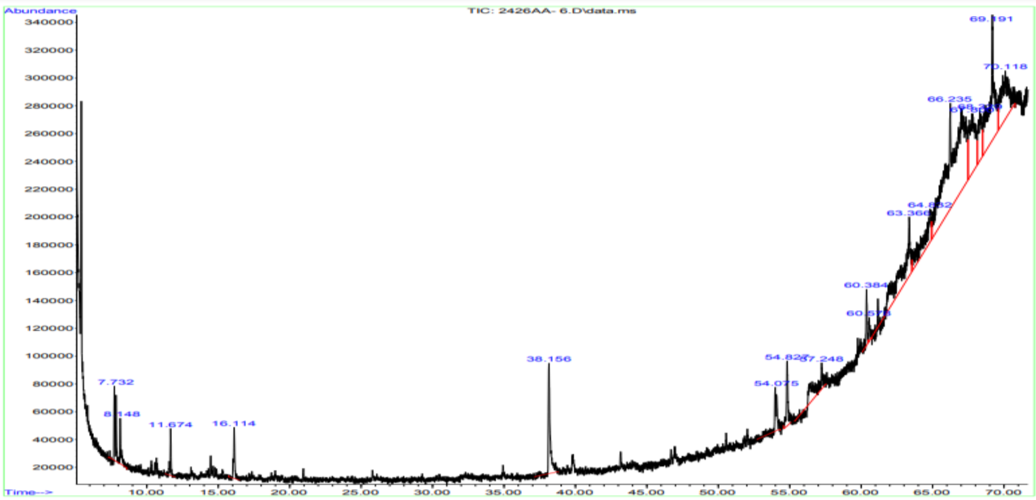

Figure 5. The chromatogram of the GC-MS analysis of the species *Launaea mucronata*

Table 7. GC-MS of the species *Senecio glaucus*

PEAK NO.	CHEMICAL COMPOUNDS	RETENTION TIME (MIN.)	AREA% 100%	MOLECULAR FORMULA	MOLECULAR WEIGHT (G/MOL)	CHEMICAL CLASSIFICATION
1	3-Hexanone	7.728	3.46	$C_6H_{12}O$	100.16	Ketone
2	2,5-Cyclohexadien-1-one, 2,6-bis(1,1-dimethylethyl)	38.151	32.96	$C_{15}H_{22}O$	218.33	Unsaturated cyclic ketone
3	Nonadecane	53.993	2.95	$C_{19}H_{40}$	268.5	Alkane
4	Eicosane, 9-octyl-	57.245	2.53	$C_{28}H_{58}$	394.8	Alkane
5	2- 2-Octadecyloxy-1,1,2,2-tetradeuteroethanol	59.972	26.22	$C_{20}H_{42}O_2$	318.6	Ether alcohol
6	Eicosane	60.389	1.97	$C_{20}H_{42}$	282.5	Alkane
7	Iron, tricarbonyl [(2,3,4, 5-.eta.)-2,3,4,5-tetrahydroxy-2,4-cyclopentadien-1-one]-	62.772	2.06	$C_8H_4FeO_8$	283.957	Organometallic compound
8	Nonyl docosanoate	67.001	10.09	$C_{31}H_{62}O_2$	466.8	Ester
9	2,2,4,5-Tetramethyl-6-(1-methyloctadecyl)-1,3-dioxan	67.573	8.61	$C_{27}H_{54}O_2$	410.7	Saturated cyclic ether compound
10	Benzo[a]heptalen-9(5H)-one, 6,7-dihydro-1,2,3,10-tetramethoxy-7-(methylamino)-, (S)-	68.219	9.15	$C_{21}H_{25}NO_5$	371.4	Polycyclic aromatic ketone

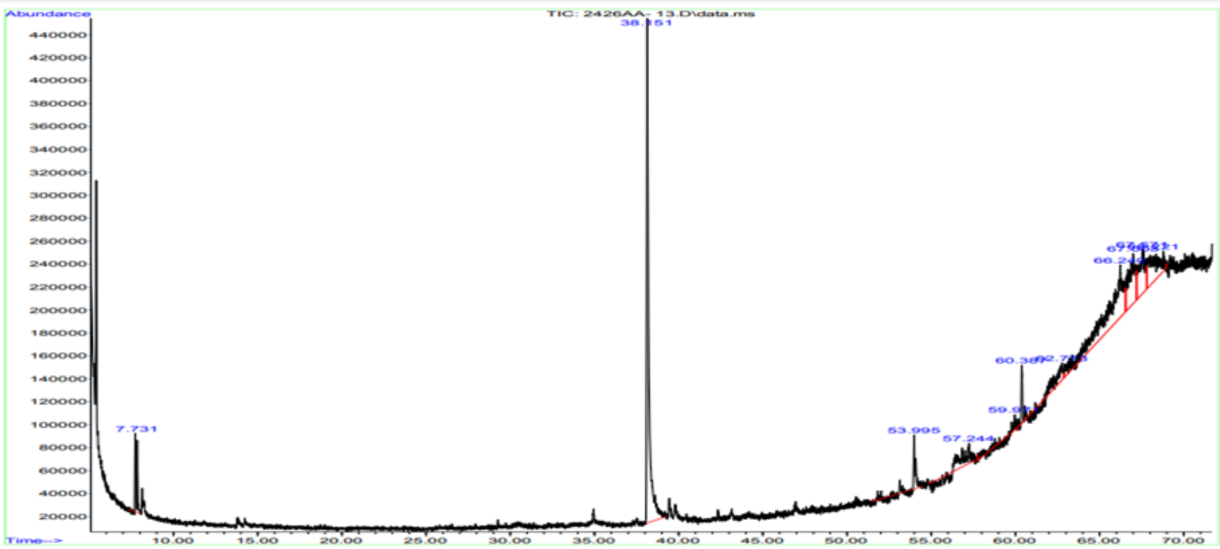

Figure 6. The Chromatogram of the GC-MS analysis of the species *Senecio glaucus*

Table 8. GC-MS of the species *Sonchus asper*

PEAK NO.	CHEMICAL COMPOUNDS	RETENTION TIME (MIN.)	AREA% 100%	MOLECULAR FORMULA	MOLECULAR- EIGHT (G/MOL)	CHEMICAL CLASSIFICATION
1	3-Hexanone	7.734	2.03	$C_6H_{12}O$	100.16	Ketone
2	Hydrazinecarboxaldehyde,methylpropylidene-,(Z)-	8.151	1.29	$C_5H_{10}N_2O$	114.15	Hydrazone
3	Nonane	11.677	0.93	C_9H_{20}	128.25	Alkane
4	Decane	16.112	1.28	$C_{10}H_{22}$	142.28	Alkane
5	2,5-cyclohexadien-1-one,2,6-bis (1 ,1-dimethylethyl)-4-methylene-	38.156	10.91	$C_{15}H_{22}O$	218.33	Unsaturated cyclic ketone
6	Nonadecane	53.999	2.03	$C_{19}H_{40}$	268.5	Alkane
7	1,2-Benzenedicarboxylic acid,bis(2-ethylhexyl)ester	54.788	2.24	$C_{24}H_{38}O_4$	390.56	Ester
8	Eicosane	60.383	42.55	$C_{20}H_{42}$	282.5	Alkane
9	Eicosyl isopropyl ether	62.578	7	$C_{23}H_{48}O$	340.6	Ether
10	Ethanone,1,1'-[3,3'-biisoxazole]-5,5'-diylbis-	63.338	14.15	$C_{10}H_8N_2O_4$	220.048	Diketone
11	Fumaric acid,2-decyl tridecyl ester	66.236	15.59	$C_{27}H_{50}O_4$	438.68	Ester

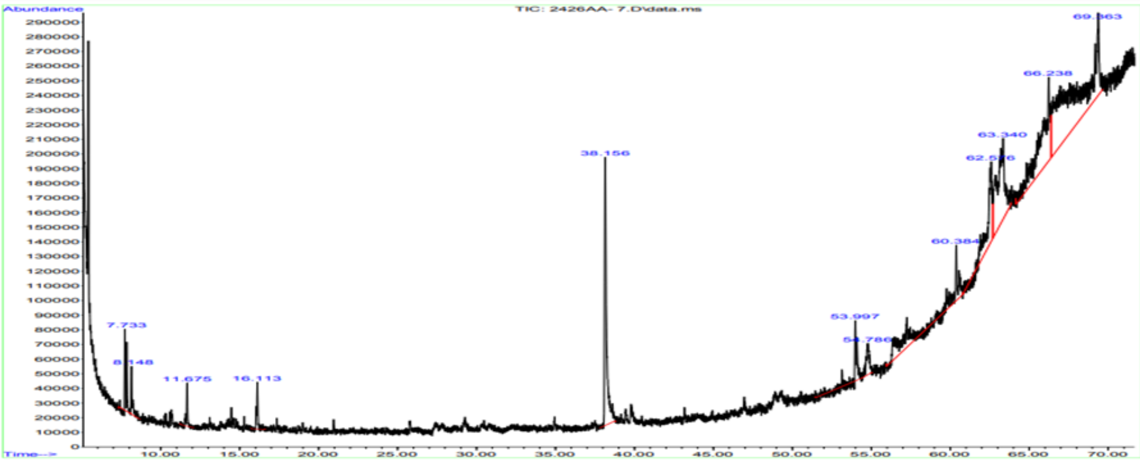

Figure 7. The chromatogram of the GC-MS analysis of the species *Sonchus asper*

Table 9. GC-MS of the species *Sonchus tenerrimus*

PEAK NO.	CHEMICAL COMPOUNDS	RETENTION TIME (MIN.)	AREA% 100%	MOLECULAR FORMULA	MOLECULAR WEIGHT (G/MOL)	CHEMICAL CLASSIFICATION
1	Nonane	11.671	1.28	$CH_3(CH_2)_7CH_3$	128.26	Alkane
2	2,5-cyclohexadien-1-one,2,6-bis (1 ,1-dimethylethyl)-4-methylene-	38.156	6.86	$C_{15}H_{22}O$	218.33	Unsaturated cyclic ketone
3	2-Heptadecanone	54.096	2.14	$C_{17}H_{34}O$	254.45	Ketone
4	Eicosyl isopropyl ether	63.361	6.69	$C_{23}H_{48}O$	340.6	Ether
5	Stigmasterol	67.527	52.9	$C29H_{48}O$	412.7	Steroid
6	(22-z)-dehydrocholesterol-1-ether	70.476	30.13	$C_{28}H_{46}O$	398.66	Ether

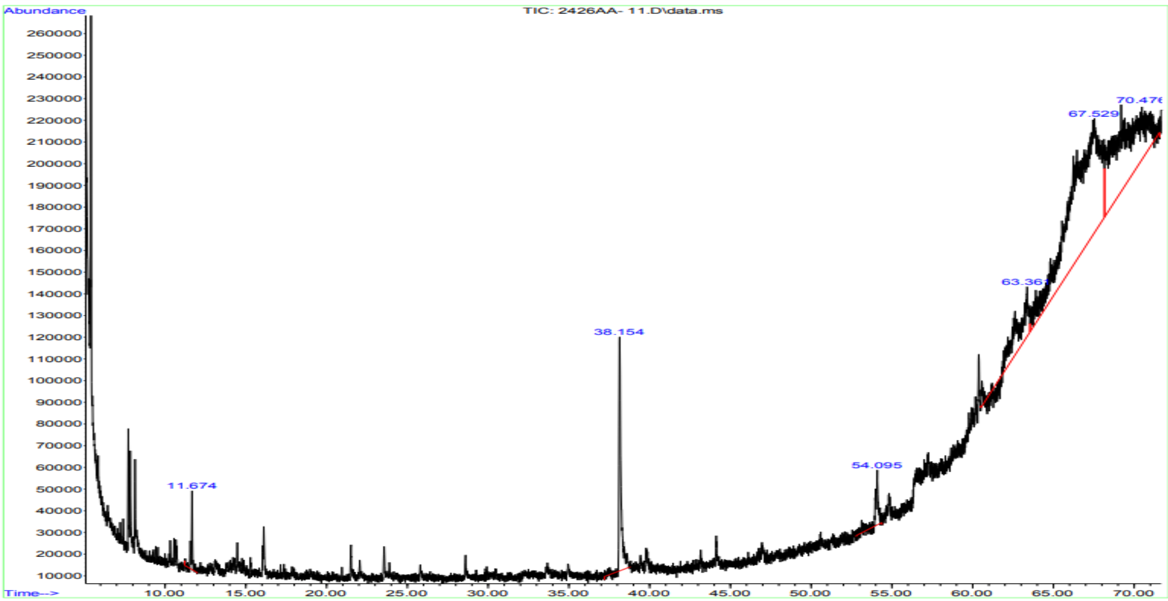

Figure 8. The chromatogram of the GC-MS analysis of the species *Sonchus tenerrimus*

HCA dendrogram analysis

The agglomerative hierarchical clustering analysis dendrogram was generated for eight taxa of Asteraceae based on 81 chemical compounds, gained by Euclidean distance using Ward's method. The dendrogram reveals two clusters graphically. The horizontal axis (Rescaled distance) represents the distance or difference between groups, and the dissimilarity within the interval is 5; the greater distance is the difference between the groups that are being merged. The vertical axis represents the studied species and the horizontal lines represent the process of merging groups. Each horizontal line indicates the merging of two groups into one larger group, and the horizontal line height represents the extent of the difference between the two merged groups. The higher line means the greater difference between the two groups. The (HCA) dendrogram illustrated in Figure 9 presents a significant correlation between the systematic classification and the chemical information as the *Carthamus tinctorius* (belongs to the cynareae tribe) is the most divergent species, as it combines at a very late stage of the analysis, indicating that it differs significantly from the other species. The dendrogram also showed a divergence between the two *Conyza* species (despite both species belonging to the Astereae tribe). However, they showed greater affinity to *Launaea mucronata* (Cichorieae tribe), which may be attributed to the fact that these species are phytoaccumulators and the presence of the compound (DEHP), which is plasticizer material in the *Conyza canadensis* is collected from a cultivated region from Baghdad, and the compound DL-Glutamic-2-d acid, N-acetyl-, dimethyl ester ($C_9H_{14}2DNO_5$) that containing Deuterium (D) in *Conyza bonariensis* which is collected from a wild region in Baghdad University campus, may indicate the role of these plants in phytoremediation, the studies have been shown that localities and environmental conditions significantly influence the phytochemical composition of these plants, resulting in comparable adaptive traits (23,27). On the other hand, *Centurea iberica* (Cardueae tribe) shows a close relation to *Conyza bonariensis*. Along with (35), the significant relations can be interpreted in understanding the biochemical origins of polymorphism in a plant species.

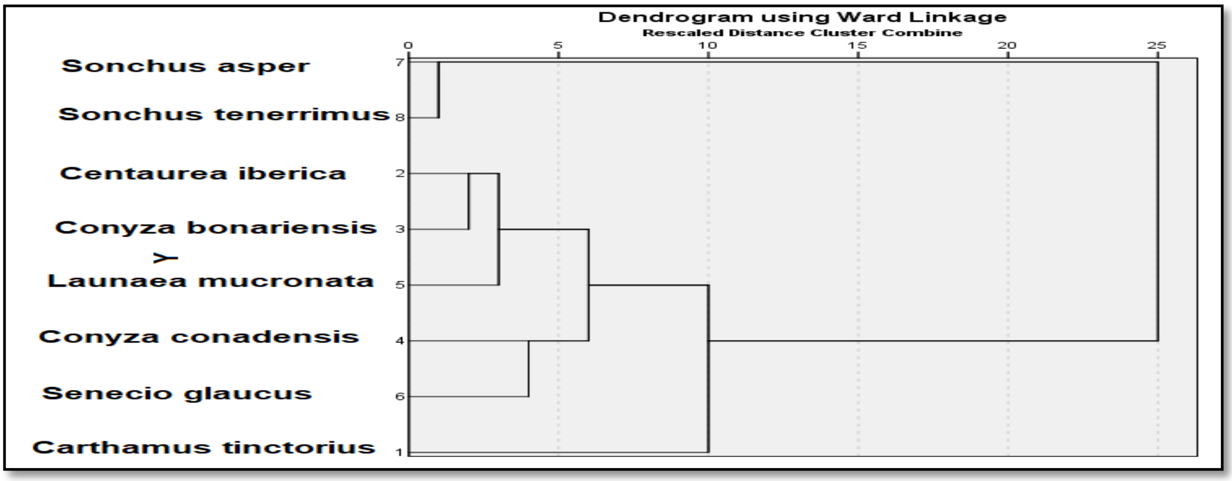

Figure 9. HCA Dendrogram of eight species of Asteraceae by using Ward's method

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