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Investigation of chemical compounds of *Astragalus galactites* (Pall.) using GC-QTOF-MS and UPC2-QTOF-MS

Chaired by **Dr. Alfredo Berzal-Herranz**
and **Prof. Dr. Maria Emília Sousa**



pharmaceuticals



Sugarjav E^{1,3*}, Gunbilig D², Irekhbayar J³, Chimedragchaа Ch¹

¹ Institute of Traditional Medicine and Technology, Ulaanbaatar, Mongolia

² Institute of Chemistry of Renewable Resources, University of Natural Resources and Life Sciences, Muthgasse 18, 1190 Vienna, Austria

³ School of Arts and Sciences, National University of Mongolia, Ulaanbaatar 14201, Mongolia

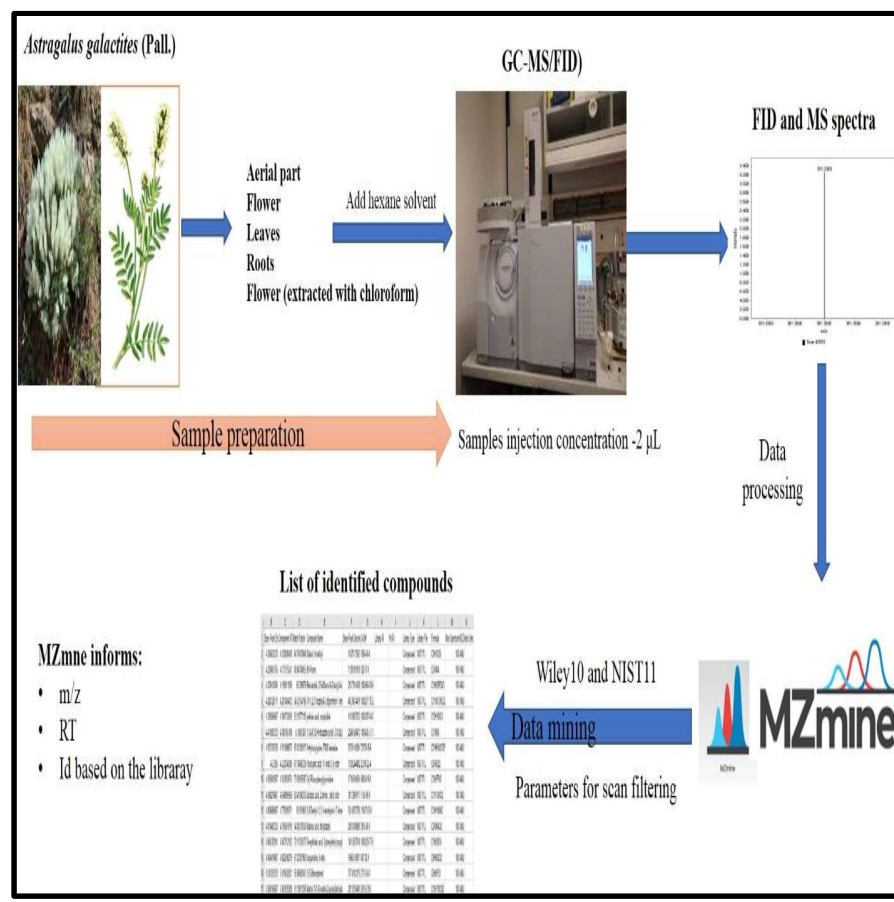
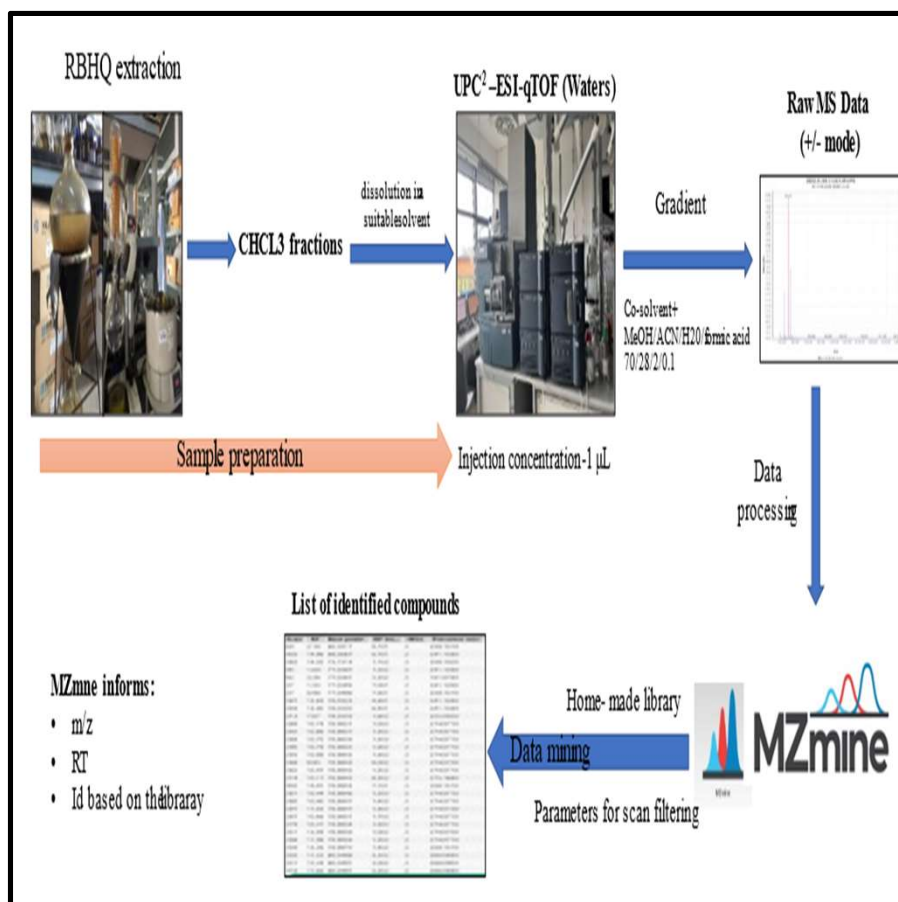
* Corresponding author: sugarjave@gmail.com





Investigation of chemical compounds of *Astragalus galactites* (Pall.) using GC-QTOF-MS and UPC2-QTOF-MS

Graphical Abstract





Abstract:

Background: We present and discuss our recent findings on the chemistry of *Astragalus galactites*. More than 20 of potentially bioactive constituents, including saponins, polyphenolic acids, polysaccharides, alkaloids, and flavonoids, were putatively identified in extracts of *A.galactites* with the aid of GC-QTOF-MS, and UPC2-QTOF-MS. This article provides a first-time such effort for the untargeted metabolite profiling of *A.galactites*.

Objective: This study aimed to shotgun analyze biological active substances in *A.galactites*, a plant used in Mongolian traditional medicine.

Material and Methods: The plant sample was collected in the Tahiltayn Mountain area (47° 91' 44" N, 106° 70' 63" E), Songino Khairhan district, Mongolia, (May 2021). Untargeted metabolite profiling analyses were performed in various plant organs (aerial parts, leaves, roots, and flowers) and previously isolated fractions (XYZ) of chloroform extract using GC-QTOF-MS and UPC2-QTOF-MS instruments.

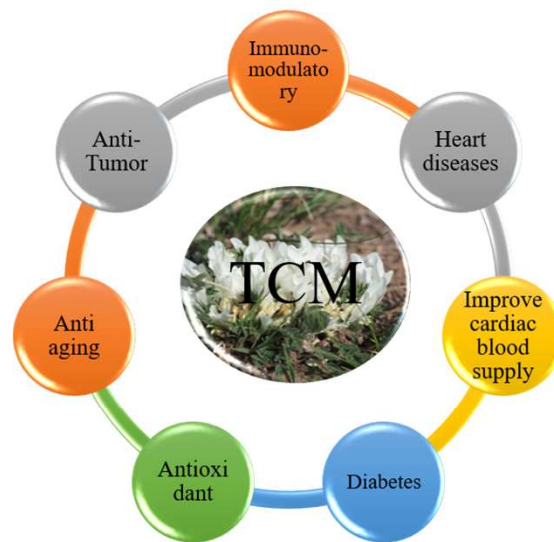
Results: Twenty-three compounds, eight phenolic acid derivatives, seven flavonoids, two diterpenoids derivatives, two monoterpenoids, one sesquiterpenoid, two fatty acids, and one lignan were identified by UPC2-QTOF-MS analysis in the chloroform fraction of *A.galactites*. Further 16 compounds, of which 14 are polysaccharide derivatives and two alkaloids were also identified putatively by GC-MS analysis in the extract of leaves, flowers, roots, and aerial parts of *A.galactites*.

Conclusion: A shotgun metabolite profiling showed the presence of numerous polyphenolic compounds, polysaccharides, and saponins to be containing in *A.galactites* samples, a medicinal plant for its anti-inflammatory properties. The presence of the above-mentioned compounds supports the pharmacological effects and radical scavenging activities we reported (XYZ) previously.

Keywords: *Astragalus galactites* Pall., GC-MS , UPC2-QTOF-MS

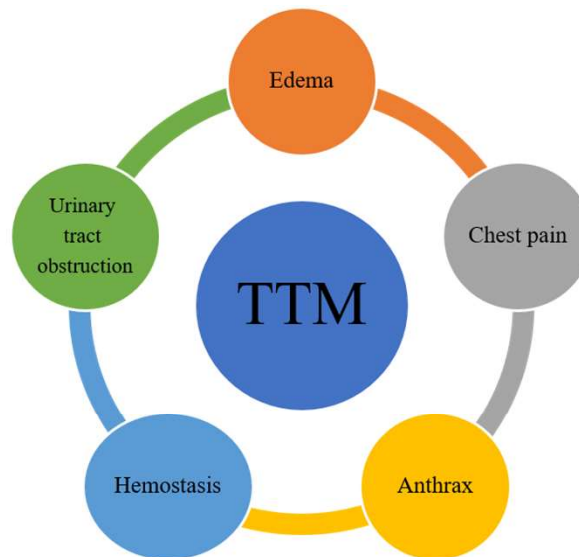


Introduction



The flowers are milky white, irregular, covered with hairs, and have small green leaves. It has no peculiar smell or bitter taste.

主编, 贾敏如, 张艺, 中国民族药词典, 中国医药科技出版社, 2015: 98



The aerial parts of *Astragalus galactites* (Pall.) are considered to be a rich source of a large amount of bioactive substances like flavonoids, alkaloids, polysaccharides and saponin

中国科学院西北高原生物研究所. 藏药志[M]. 西宁: 青海人民出版社, 1991:444-445.

А.Азирмаа, М.Амбара, Г.Пүрэвсүрэн, 1991

Лигиаа У. Монгол орны эмийн ургамлыг өрнө дорнын анагаах ухаанд хэрэглэхүй. 2005 он. х. 30, 453-454.



Research purpose

- This study aimed to shotgun analyze biological active substances in *A. galactites*, a plant used in Mongolian traditional medicine.

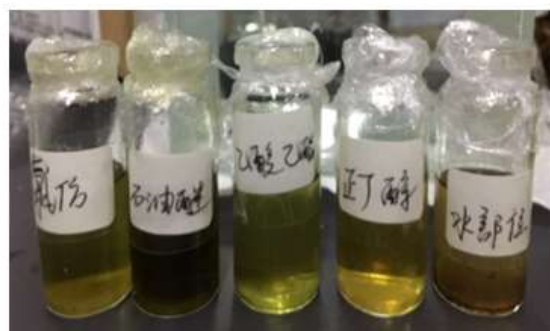
Research material

- The plant sample was collected in the Tahiltayn Mountain area (47° 91' 44" N, 106° 70' 63" E), Songinokhairhan district, Mongolia, (May 2021).
- *Astragalus galactites* (Pall.) is a native species to the northern part of China, Mongolia, and Siberia.





Results and discussion



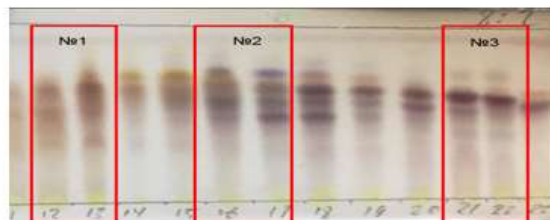
Chloroform fraction, 10g



Sephadex LH-20



1-30 fractions



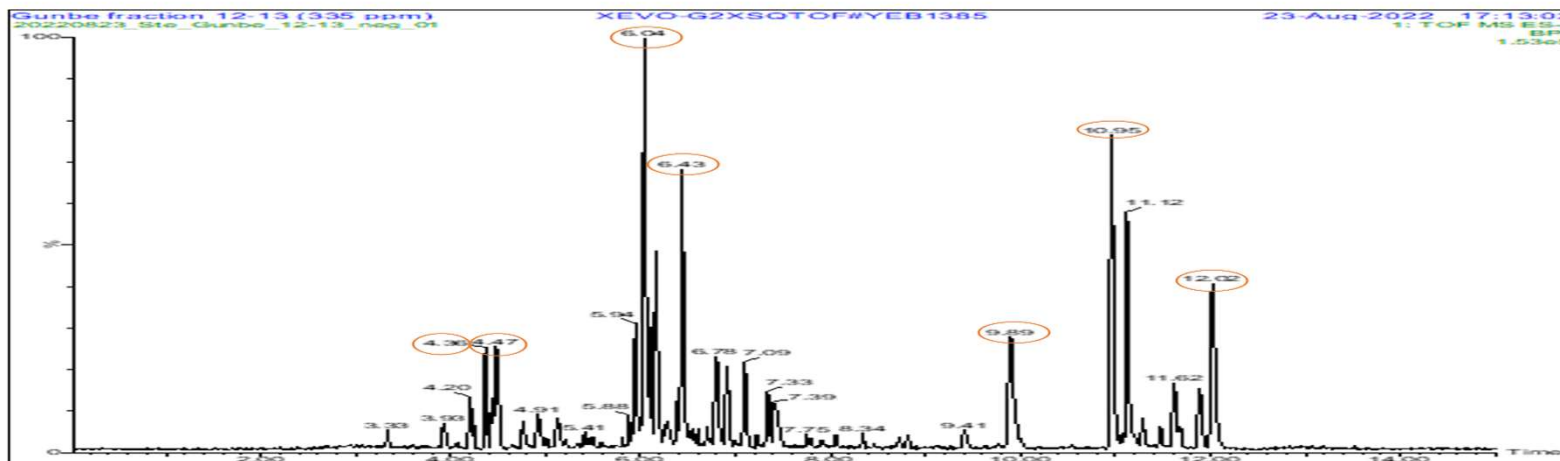
TLC analysis

No	Parameters	Condition
1	System	ACQUITY UPC ²
2	Detector	PDA
3	Mobile phase A	CO ₂
4	Mobile phase B	MeOH/ACN/H ₂ O/formic acid 70/28/2/0.1
5	Flow rate	1.2 mL/min 毫升/分钟
6	Pressure	2001.0 psi
7	Run time	15 min
8	Wavelength	UV 230-700 nm
9	Column temperature	45 °C
10	Sample temperature	20 °C

No	Time (min)	Flow rate	%A	%B	Curve
1	Initial	1.200	99.0	1.0	Initial
2	1.00	1.200	99.0	1.0	6
3	10.00	1.200	70.0	30.0	6
4	10.50	1.200	60.0	40.0	6
5	11.50	1.200	60.0	40.0	6
6	12.00	1.200	99.0	1.0	6
7	15.00	1.200	99.0	1.0	6



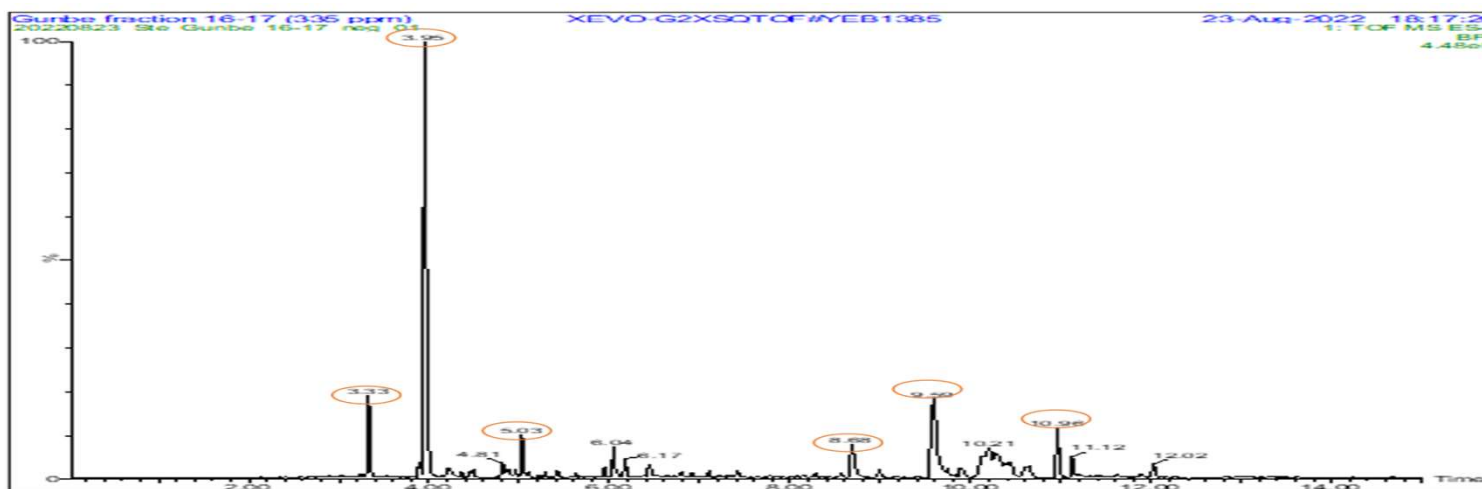
UPC²-Q-TOF-MS/MS spectrum of Fraction-1



No	m/z	RT /min/	Compounds name	Chemical formula	Class of compound
1	225	4.36	Dihydrosinapic acid	C ₁₁ H ₁₄ O ₅	Phenolic acids
2	223	4.47	Sinapic acid	C ₁₁ H ₁₂ O ₅	Phenolic acids
3	291	6.04	Methyl pinolenate	C ₁₉ H ₃₂ O ₂	Fatty acid
4	305	6.43	(+)-Gallocatechin	C ₁₅ H ₁₄ O ₇	Flavonoids
5	178	9.89	Hippuric acid	C ₉ H ₉ NO ₃	Phenolic acids
6	289	10.95	Catechin	C ₁₅ H ₁₄ O ₆	Polyphenol
7	303	12.02	3'-O-Methylcatechin	C ₁₆ H ₁₆ O ₆	Flavonoids



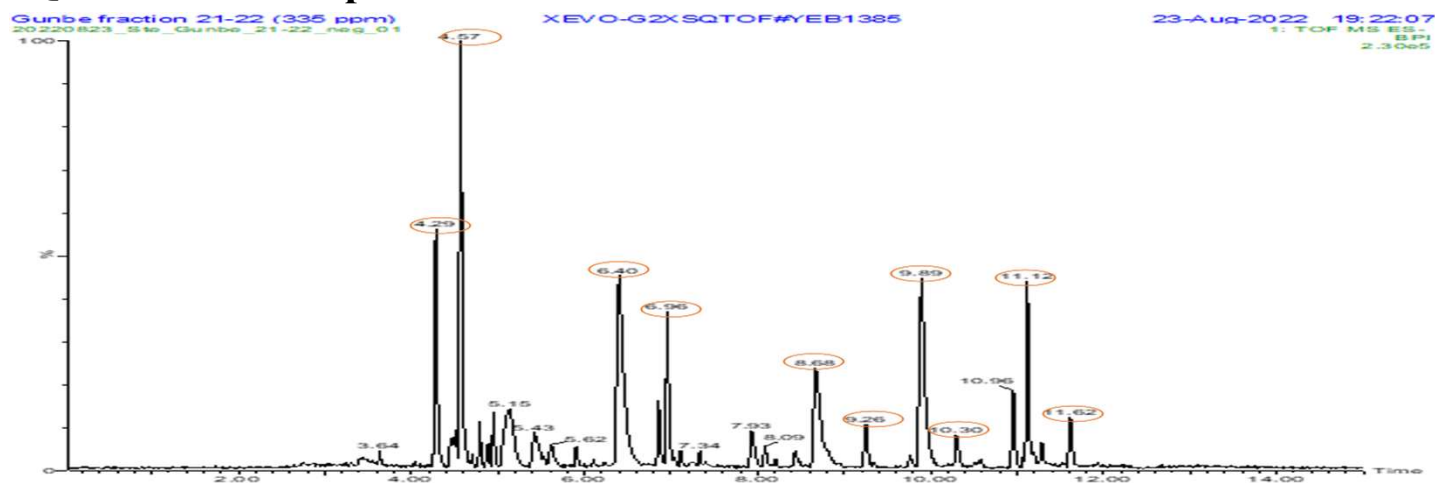
UPC²-Q-TOF-MS/MS spectrum of Fraction-2



No	m/z	RT /min/	Compounds name	Chemical formula	Class of compound
1	221	3.33	Alpha-bisabolol	C ₁₅ H ₂₆ O	Sesquiterpenoids
2	195	3.95	Hydroxycaffeic acid	C ₉ H ₈ O ₅	Phenolic acids
3	178	5.03	Hippuric acid	C ₉ H ₉ NO ₃	Phenolic acids
4	419	5.68	Apigenin 7-O-glucoside	C ₂₁ H ₂₄ O ₉	Flavonoids
5	579	9.59	Naringin	C ₂₇ H ₃₂ O ₁₄	Flavonoids
6	289	10.96	Manool	C ₂₀ H ₃₄ O	Diterpenes



UPC²-Q-TOF-MS/MS spectrum of Fraction-3



No	m/z	RT /min/	Compounds name	Chemical formula	Class of compound
1	151	4.29	cis-verbenol	C ₁₀ H ₁₆ O	Monoterpenoids
2	135	4.57	gamma-terpinene	C ₁₀ H ₁₆	Monoterpene
3	195	6.40	Dihydroferulic acid	C ₁₀ H ₁₂ O ₄	Phenolic acids
4	313	6.96	Irisolidone	C ₁₇ H ₁₄ O ₆	Flavonoids
5	433	8.68	Quercetin 3-O-arabinoside	C ₂₀ H ₁₈ O ₁₁	Flavonoids
6	359	9.26	(+)-lariciresinol	C ₂₀ H ₂₄ O ₆	Lignans
7	178	9.89	Hippuric acid	C ₉ H ₉ NO ₃	Phenolic acids
8	519	10.30	5,3',4'-Trihydroxy-3-methoxy-6:7-methylenedioxy flavone 4'-O-glucuronide	C ₂₃ H ₂₀ O ₁₄	Flavonoids
9	289	11.12	13-epi-manoyl oxide	C ₂₀ H ₃₄ O	Diterpenes
10	305	11.62	7,11,14-Eicosatrienoic acid (Et) C ₂₀ :3	C ₂₀ H ₃₄ O ₂	Fatty acid

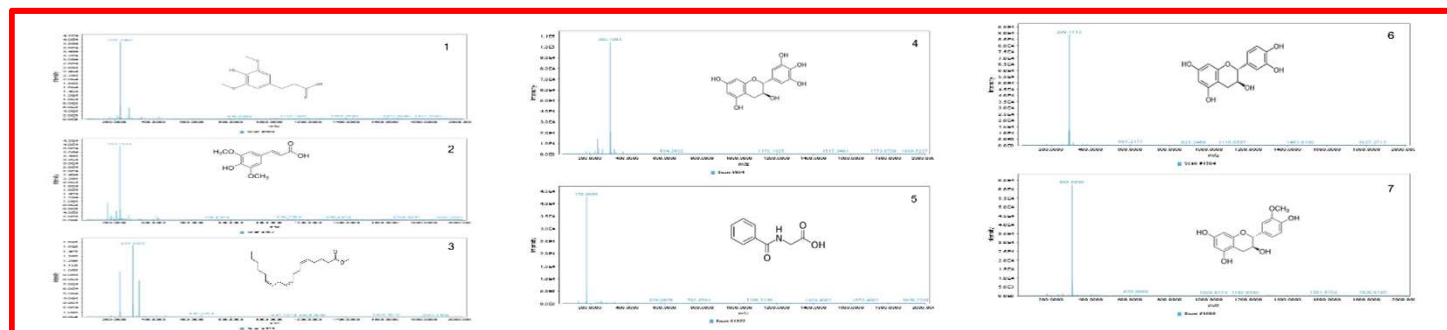


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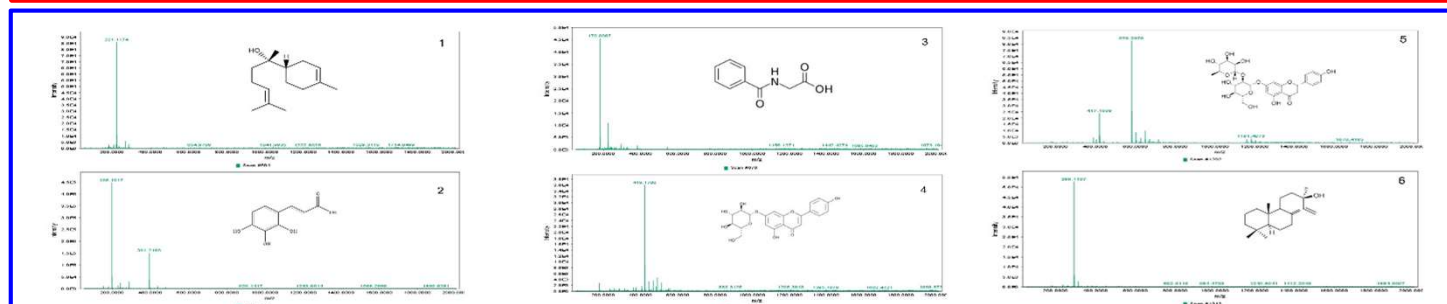
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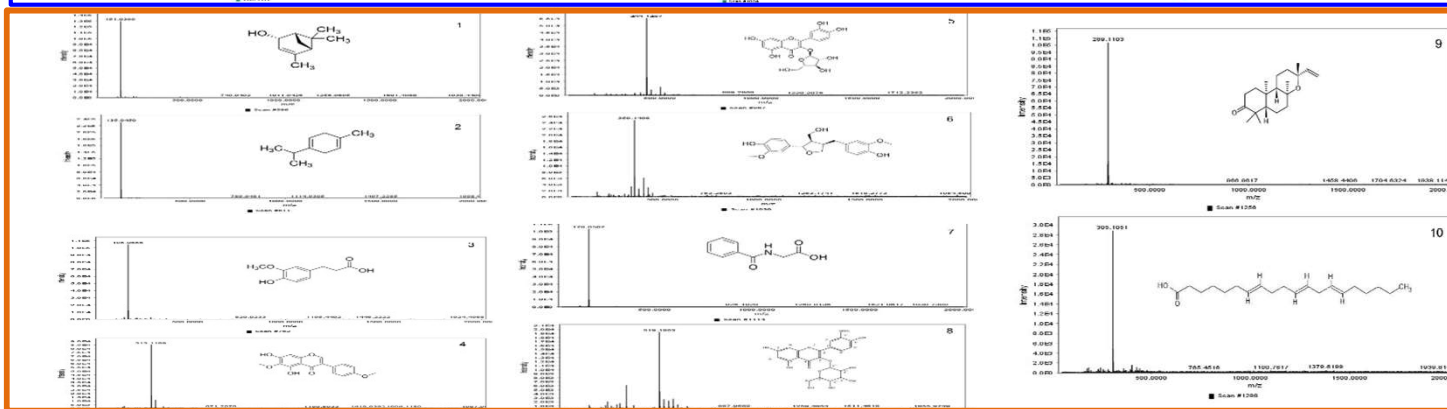
Fraction-1



Fraction-2



Fraction-3



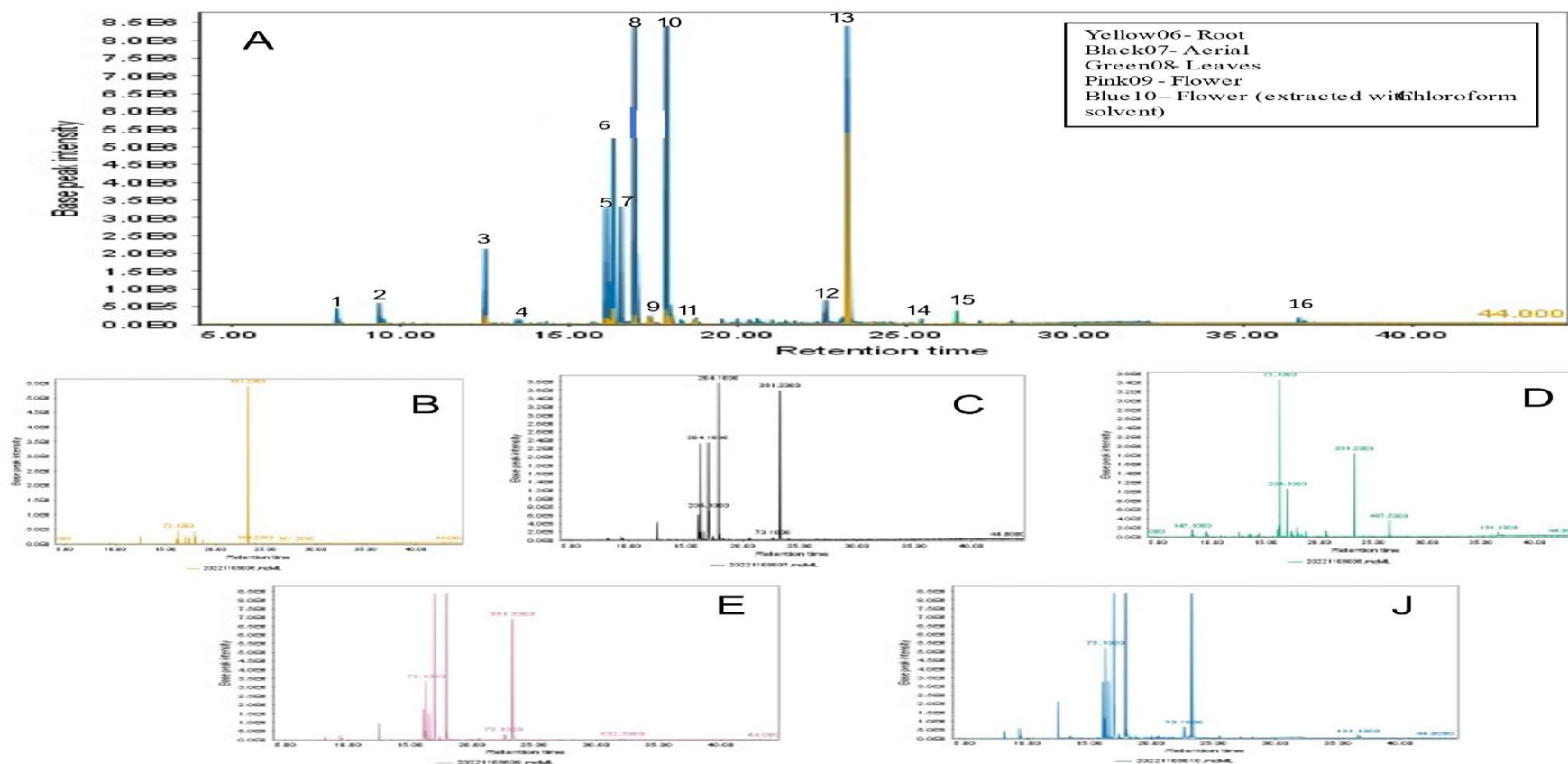


Figure 1. GC-MS total ion chromatogram of *Astragalus galactites* (5 groups)

A-GC-MS total ion chromatogram of aerial (black), flower (pink), root (yellow), leaves (leaves), flower (extracted with chloroform) (blue), B- root (yellow06), C- aerial (black07), D-leaves (green08), E-flower (pink09), J-flower (extracted with chloroform solvent-blue10)



GC-MS analysis of *A. Galactites*

No	Peak RT ^a (min)	Compound detected*	Molecular Formula	Part of the plant
1	8.319517	N-Benzyl-1H-benzimidazole	C ₁₄ H ₁₂ N ₂	Aerial, Leaves, Flower, Flower ^b
2	9.4346177	Silanol, trimethyl-, phosphate	C ₉ H ₂₇ O ₄ PSi ₃	Root, Flower ^b , Leaves, Aerial, Flower
3	12.5485025	Malic acid, 3TMS derivative	C ₁₃ H ₃₀ O ₅ Si ₃	Root, Flower ^b , Aerial, Flower
4	13.482329	2,3,4-Trihydroxybutyric acid tetrakis (trimethylsilyl), Threonic acid	C ₁₆ H ₄₀ O ₅ Si ₄	Leaves, Flower ^b
5	16.112684	D-(-)-Fructofuranose, pentakis(trimethylsilyl) ether (isomer 2)	C ₂₁ H ₅₂ O ₆ Si ₅	Root, Flower ^b , Aerial, Flower
6	16.328128	D-Pinitol, pentakis(trimethylsilyl) ether	C ₂₂ H ₅₄ O ₆ Si ₅	Root, Aerial, Leaves, Flower, Flower ^b
7	16.555017	β-D-Galactofuranose	C ₂₁ H ₅₂ O ₆ Si ₅	Root, Aerial, Flower, Flower ^b
8	16.953380	D-(+)-Galactopyranose, 5TMS derivative	C ₂₁ H ₅₂ O ₆ Si ₅	Root, Aerial, Leaves, Flower, Flower ^b
9	17.403437	D-Sorbitol, 6TMS derivative	C ₂₄ H ₆₂ O ₆ Si ₆	Root, Aerial, Leaves, Flower
10	17.878917	β-D-Glucopyranose, 5TMS derivative	C ₂₁ H ₅₂ O ₆ Si ₅	Root, Aerial, Leaves, Flower, Flower ^b
11	18.760181	Myo-Inositol, 6TMS derivative	C ₂₄ H ₆₀ O ₆ Si ₆	Root, Aerial Leaves, Flower, Flower ^b
12	22.504929	Docosanol, TMS derivative	C ₂₅ H ₅₄ O _{Si}	Aerial, Flower, Flower ^b
13	23.247551	Sucrose, 8TMS derivative	C ₃₆ H ₈₆ O ₁₁ Si ₈	Root, Aerial, Flower, Flower ^b
14	25.460362	Silane,dimethyl(4-(2-phenylprop-2-yl)phenoxy) decyloxy-	C ₂₇ H ₄₂ O ₂ Si	Leaves, Flower ^b
15	26.442339	1-[(4-Methylbenzene) sulfonyl]pyrrole	C ₁₁ H ₁₁ NO ₂ S	Leaves
16	36.521192	D- (+)-Cellobiose, octakis(trimethylsilyl) ether, methyloxime	C ₃₇ H ₈₉ NO ₁₁ Si ₈	Leaves, Flower ^b

*The compounds that were identified and compared with a similar mass fragmentation in the NIST database library. a R.T: Retention time; b Flower: Sample of flower extracted with chloroform solvent



Conclusions

In summary, polyphenolic compounds, polysaccharides, and saponins are the main compounds of *A. Galactites* medicinal plants with anti-inflammatory properties, and these biologically active compounds are explained by the pharmacological effects and radical scavenging activities that we have previously investigated. In the future, we are focused on researching and developing of new herbal medicines for anti-immune and gouty arthritis.



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