Scientific Papers. Series B, Horticulture. Vol. LXIX, No. 1, 2025
Print ISSN 2285-5653, CD-ROM ISSN 2285-5661, Online ISSN 2286-1580, ISSN-L 2285-5653

THE CHEMICAL COMPOSITION OF THE ESSENTIAL OIL AND ASSOCIATED HYDROSOL OBTAINED FROM TWO PLANTS OF THE ASTERACEAE FAMILY, *SANTOLINA CHAMAECYPARISSUS* L. AND *TANACETUM VULGARE* L.

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Abstract

The use of plants throughout the centuries has been essential for the survival and development of human civilizations. Plants have been used in multiple fields, such as food, medicine, construction, religion, and even in art and culture. In recent years, natural compounds have attracted considerable attention in various fields due to their wide-ranging biological activities. Essential oils and their associated hydrosols, in particular, are being explored for their ability to control plant pests, as well as their, antimycotic and antiparasitic effects. These substances are typically faster and more cost-effective to produce, and are generally considered safer for the environment and non-target organisms than conventional pesticides. Earlier studies have demonstrated that the primary components found in the essential oil of Tanacetum vulgare L. were oxygenated monoterpenes, including compounds like camphor, trans-chrysantenyl acetate, cis-verbenol, thujone, eucalyptol, and α-campholenal. For Santolina chamaecyparissus L., the primary components identified were artemisia ketone, camphor, and beta-phellandrene.
This study highlights the chemical composition of the essential oil and associated hydrosol obtained from two plants of the Asteraceae family, Santolina chamaecyparissus L. and Tanacetum vulgare L .

Key words: *chemical composition , essential oil, hydrosol, Santolina chamaecyparissus, Tanacetum vulgare.*

INTRODUCTION

The use of plants has been pivotal for the survival and advancement of human civilizations over centuries. They have served diverse purposes, including food, medicine, construction, religion, art, and culture. In recent years, natural compounds have garnered significant attention across various fields due to their broad biological activities. Essential oils and their corresponding hydrosols, in particular, are being investigated for their potential to control plant pests and their antimycotic and antiparasitic properties. These natural substances are generally faster and more cost-effective to produce and are considered safer for both the environment and non-target organisms compared to conventional pesticides.

This study focuses on analyzing the chemical composition of the essential oil and hydrosol extracted from two Asteraceae family plants: *Santolina chamaecyparissus* L. and *Tanacetum vulgare* L..

The genus *Santolina* (family Asteraceae) is a taxonomically intricate group of plant species found extensively throughout the Mediterranean region. *Santolina chamaecyparissus* L., commonly known as cotton lavender, is a resilient, aromatic, evergreen shrub characterized by its dense mound of appealing grayish-silver foliage. Renowned for its biological properties, it has been utilized in traditional medicine since ancient times.

Some species of *Santolina chamaecyparissus* L. has been studied for its oil constituents (Senatore F., 1994; Perez-Alonso M. J. and Negueruela, 1988). Research indicates that its chemical composition varies depending on factors such as origin and season (Derbesy M., 1982; Brunke E.J., 1992; Perez-Alonso M. J., 1992; Giner R. M., 1993; Lawrence B. M., 1995; Vernin G., 1991).

Several subspecies of *Santolina chamaecyparissus* L. originating from Spain have been reported to primarily contain 1,8-cineole (2-18%), artemisia ketone (0.1-28%), camphor (trace - 43%), borneol (1-28%), copaenol (trace - 15%), cubenol (1-17%), and alloaromadendrene (19%) as their major constituents (Villar A., 1986; Perez-Alonso M. J., 1992).
The essential oil of *Santolina chamaecyparissus* L. from French origin primarily contained artemisia ketone, myrcene, and β-phellandrene as its major constituents (Derbesy M., 1982; Giner R. M., 1993; Lawrence B. M., 1995). In contrast, the oil from a cultivar of *Santolina chamaecyparissus* L. was characterized by longiverbenone (9-18%) in addition to artemisia ketone (8-34%) and β-phellandrene (8-18%) as key components. *Santolina chamaecyparissus* L. is notable for its intriguing fragrance, making it valuable to the perfume industry, and its oil holds commercial importance in France.
In Turkey studies revealed that the major compounds were : artemisia ketone (38.1%), camphor (11.7%), β-phellandrene (9.2%), α-bisabolol (6.6%) and myrcene (4.3%) (Demirci B., 2000).
Tanacetum vulgare L. is a perennial, herbaceous flowering plant belonging to the genus *Tanacetum* in the Asteraceae family. Native to temperate regions of Europe and Asia, it has also been introduced to other parts of the world, including North America, where it has become invasive in certain areas. Commonly referred to as common tansy, bitter buttons, cow bitter or golden buttons.
Numerous species of *Tanacetum* L. have been studied for the biological activities of their metabolites, including anti-inflammatory (Kwok BHB, 2001; Dornelles VCM. 1998), anti-migraine (Dornelles VCM., 1998), anti-ulcerogenic (Tournier H., 1998), cytotoxic (Goren N., 1996), antifeedant (Goren N., 1994) and antibacterial properties (Goren N., 1992). The genus comprises approximately 200 species, primarily distributed across Europe and western Asia (Heywood VH., 1976). Some species, such as tansy (*T. vulgare*), Dalmatian insect flower (*T. cinerariifolium*), and feverfew (*T. parthenium*), are particularly well-known.
The roots, leaves, and flowers of the two most extensively studied species, *Tanacetum vulgare* L. and *Tanacetum parthenium* L. Sch. Bip. ex Oliv., are abundant in sesquiterpene lactones (such as parthenolide, tanacetin, and tanacetols), tannins, and flavonoids (Bruni A., 2009).
Research into the chemical composition of essential oils from various *Tanacetum* species has revealed significant variability (Mockute D., 2004; Rohloff J., 2004; Keskitalo M., 2001; Chanotiya CS., 2007). These studies identified camphor, α- and β-thujone, carvone, pinocarvone, borneol, bornyl acetate, and 1,8-cineole as major constituents of the oils. A comprehensive review by Lawrence (Lawrence BM., 2000) of studies on *T. vulgare* oil composition published up to 1996 classified tansy oils into 23 chemotypes based on their primary components. Additionally, it was noted that commercial tansy oils are predominantly of the thujone type. Thujone is recognized as a bioactive compound with medicinal properties but exhibits toxicity at high concentrations. The essential oils of 40 *T. vulgare* samples from Lithuania were analyzed and grouped into four categories, with 1,8-cineole and camphor chemotypes being the most prevalent (Judzentiene A., 2005).

MATERIALS AND METHODS

Plant material from *Santolina chamaecyparissus* L. was harvested from a garden in Constanța, Romania (44°10′24″N 28°38′18″E), in August 2024.
For *Tanacetum vulgare* L., the plant material was collected from the wild flora in the Viscri area, Brașov, Romania (46°3′24″N 25°5′49″E), in August 2024. Both the essential oil and hydrosol were extracted from dried plant material.
For both species, the entire plant, including the stems, leaves, and inflorescences, was used.
Various methods can be used to obtain essential oils and hydrosols, such as water distillation techniques, cold pressing, supercritical CO_2 extraction, Soxhlet extraction, and newer approaches like microwave- and ultrasonic-assisted extractions. The goal is to extract volatile compounds from plants, which are present in smaller amounts but provide significant value. Water distillation remains the traditional method for essential oils and hydrosols production, representing 93% of the

total production. Two main techniques can be used, depending on how water interacts with the aromatic plants during extraction: hydro distillation or steam distillation . This process results in two immiscible phases during condensation, with the aqueous phase byproduct referred to as "hydrosol" (Degirmenci, H., 2020; de Elguea-Culebras, G.O., 2022; Tang, M., 2021; Timung, R., 2016; Traka, C.K., 2018).
Oil and hydrosol samples were analyzed without any other preparation or dilution. 1 µL of sample was injected in the gas-chromatographic system coupled with mass spectrometer (GC-MS, Perkin Elmer Clarus 680/SQ 8T, Perkin Elmer, CT, USA) equipped with an Elite-5MS capillary column (30 m x 0.25 x 0.25 µm (Perkin Elmer, CT, USA), using helium as carrier gas (flow rate of 1.0 mL/min). The temperature program was as follows: initial temperature: 40°C, initial hold time 2min, increase by 10°C/min to 300°C, hold time 2 min. The injection was performed in split mode (split ratio 50:1 for hydrosol and 200:1 for oil sample), and the injector temperature was set to 200°C. The MS operating conditions were: source temperature 210°C, transfer line temperature 310°C, electron impact ionization EI+ at 70eV and a solvent delay of 3 min. The qualitative analysis was performed using NIST Library, version 2017 and Wiley Library, version 9.0.
For each sample, 30 most abundant peak areas were included in the library search. A threshold for spectra match of 700 (70% probability) was chosen to determine which compounds are present in the sample analyzed.

RESULTS AND DISCUSSIONS

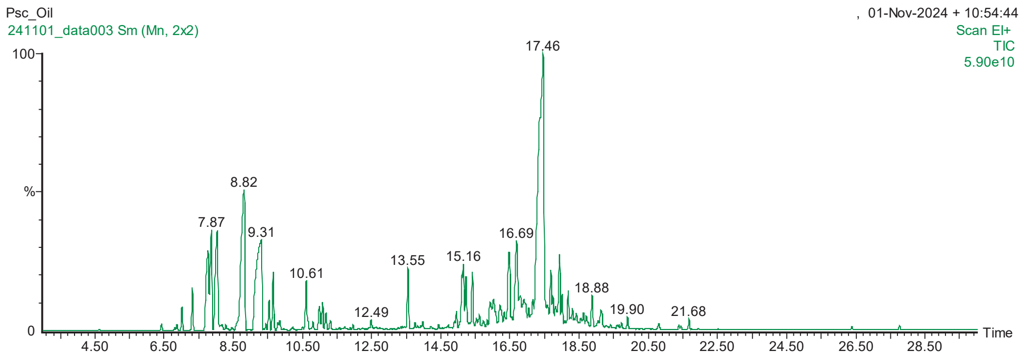
The chemical composition of *Santolina chamaecyparissus* L. essential oil was analyzed, revealing its complexity, with variations in the ratio (Table1, Figure1).

Table 1. *Santolina chamaecyparissus* L. essential oil compounds

	Compound name	Retention time (min)	Probability (%)	CAS #	Area	% from the sum of areas
1	à-PINENE (-)-	7.00	92.4	80-56-8	91444856	0.88
2	Camphene	7.31	93.2	79-92-5	182800224	1.76
3	à-PINENE	7.72	80.6	80-56-8	656930816	6.33
4	2-a-Pinene	7.82	84.4	127-91-3	670512192	6.46
5	a-Myrcene	7.99	68.9	123-35-3	776015936	7.48
6	Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1à,2à,5à)-	8.75	72.8	17699-16-0	1536558464	14.81
7	3-Butyn-1-ol	9.16	62.3	927-74-2	1637742208	15.79
8	1,5-Heptadien-4-ol, 3,3,6-trimethyl-	9.47	86.0	27644-04-8	85404568	0.82
9	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	9.59	90.6	586-62-9	149126032	1.44
10	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	10.57	93.1	464-48-2	150287424	1.45
11	endo-Borneol	10.95	92	507-70-0	62799712	0.61
12	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)- (CAS)	11.05	81.4	562-74-3	66607784	0.64
13	2-Cyclohexen-1-one, 4-(1-methylethyl)-	11.15	91.2	500-02-7	50927672	0.49
14	1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethyl)-	12.47	84	21391-98-0	11364010	0.11
15	Tricyclo[5.4.0.0(2,8)]undec-9-ene, 2,6,6,9-tetramethyl-, (1R,2S,7R,8R)-	13.53	91	5989-08-2	208374032	2.01
16	AROMADENDRENE	14.95	88.7	489-39-4	43160140	0.42
17	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl- (CAS)	15.12	90	644-30-4	189657248	1.83
18	GERMACRENE-D	15.20	90.8	23986-74-5	185693184	1.79

	Compound name	Retention time (min)	Probability (%)	CAS #	Area	% from the sum of areas
19	(1S,2E,6E,10R)-3,7,11,11-Tetramethylbicyclo[8.1.0]undeca-2,6-diene	15.38	89.6	24703-35-3	169193424	1.63
20	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1aà,4aà,7á,7aá,7bà)]-	16.39	85.3	6750-60-3	145673600	1.40
21	(-)-Caryophyllene oxide	16.45	86.8	1139-30-6	220750816	2.13
22	8-Isopropenyl-1,3,3,7-tetramethyl-bicyclo[5.1.0]oct-5-en-2-one	16.63	76.1	-	304379168	2.93
23	Longiverbenone	17.31	77.8	64180-68-3	2491115264	24.01
24	((4aS,8S,8aR)-8-Isopropyl-5-methyl-3,4,4a,7,8,8a-hexa-hydronaphthalen-2-yl)methano	17.86	79.3	135118-51-3	130993424	1.26
25	3-(1-Naphthyl)pentane	18.83	82.2	3042-56-6	86161184	0.83
26	2(1H)-Naphthalenone, octahydro-4a-methyl-7-(1-methylethyl)-, (4aà,7á,8aá)-	20.78	68.3	54594-42-2	20530308	0.20
27	Kaur-16-ene (CAS	21.37	91.3	562-28-7	11904855	0.11
28	1-Octadecanol	21.44	88.5	112-92-5	6803466	0.07
29	Phytol	21.67	87.9	150-86-7	26131014	0.25
30	Pentatriacontane (CAS)	26.39	84.9	630-07-9	5995508	0.06

Total ion chromatogram recorded (TOC)



*Psc oil - Plant *Santolina chamaecyparissus* L. essential oil

Figure 1. *Santolina chamaecyparissus* L. essential oil TOC

The compound longiverbenone is the most abundant, contributing 24.01% of the total area. This suggests that longiverbenone is the dominant compound in this sample and could significantly influence the oil's aroma and bioactivity.

Other significant compounds include:3-butyn-1-ol (15.79%), bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)- (14.81%), bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S)- (15.43%), (1S,2E,6E,10R)-3,7,11,11-tetramethylbicyclo[8.1.0]undeca-2,6-diene (1.63%).

These compounds are major contributors to the chemical composition of the oil and could play a role in its fragrance and therapeutic effects.

A significant presence of terpenes and sesquiterpenes, such as α-pinene, camphene, myrcene, and caryophyllene oxide, indicates that the oil likely has strong aromatic properties and may have biological activities such as anti-inflammatory or antimicrobial effects.

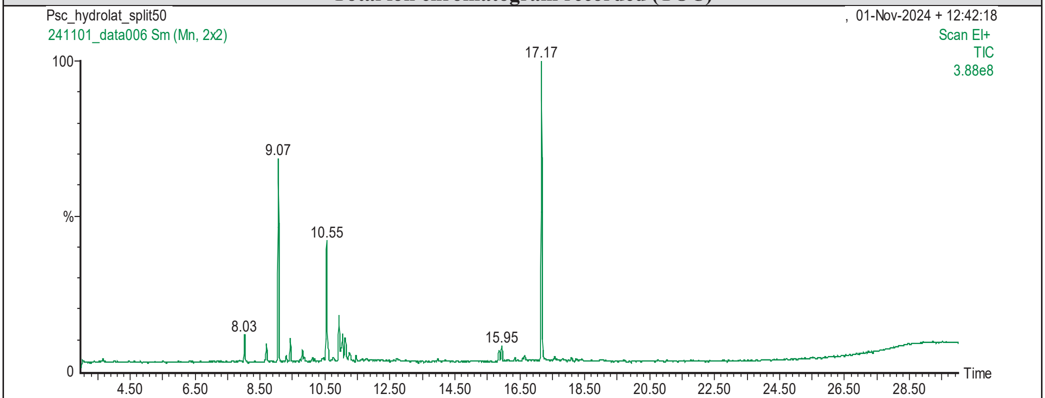
The oil contains a wide variety of functional groups, including alcohols, ketones, aldehydes, and hydrocarbons, which suggests that the oil may have complex chemical interactions. These components may contribute to its bioactive properties, such as potential antimicrobial, anti-inflammatory, or antioxidant effects.

Analyses of *Santolina chamaecyparissus* L. hydrosol revealed that longiverbenone is the most abundant, accounting for 40.88% of the total area (Table 2, Figure 2).

Table 2. *Santolina chamaecyparissus* L. hydrosol compounds

	Compound name	**Retention time (min)**	**Probability (%)**	**CAS #**	**Area**	**% from the sum of areas**
1	2,5,5-trimethyl-3,6-heptadien-2-ol	8.03	87.9	26127-98-0	1308652	3.66
2	1,5-Heptadien-4-one, 3,3,6-trimethyl- (CAS)	9.07	92.3	546-49-6	9340579	26.11
3	1,5-Heptadien-4-ol, 3,3,6-trimethyl-	9.44	84.1	27644-04-8	1178120	3.29
4	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	10.55	94.1	464-48-2	5520606	15.43
5	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S-endo)-	10.94	90.9	464-45-9	1869845	5.23
6	Terpinen-4-ol	11.05	85.5	562-74-3	1050179	2.94
7	2-Cyclohexen-1-one, 4-(1-methylethyl)-	11.14	80.9	500-02-7	879902	2.46
8	Longiverbenone	17.18	82.9	64180-68-3	14623996	40.88

Total ion chromatogram recorded (TOC)



*Psc hydrosol – Plant *Santolina chamaecyparissus* L. hydrosol

Figure 2. *Santolina chamaecyparissus L. hydrosol* TOC

This suggests that longiverbenone is the major contributor to the *Santolina chamaecyparissus* L. hydrosol's chemical profile and may have a significant influence on its aroma and bioactivity.

Several important terpenoid compounds are identified, such as bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- (15.43%) and bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl- (5.23%). These compounds contribute to the distinctive aroma and may have antimicrobial or other bioactive properties, which are common for compounds found in essential oils and hydorsols.

The presence of oxygenated compounds like terpinen-4-ol (2.94%) and 2-cyclohexen-1-one, 4-(1-methylethyl)- (2.46%) indicates that the hydrosol may also have therapeutic properties, including anti-inflammatory, antimicrobial, or antifungal effects.

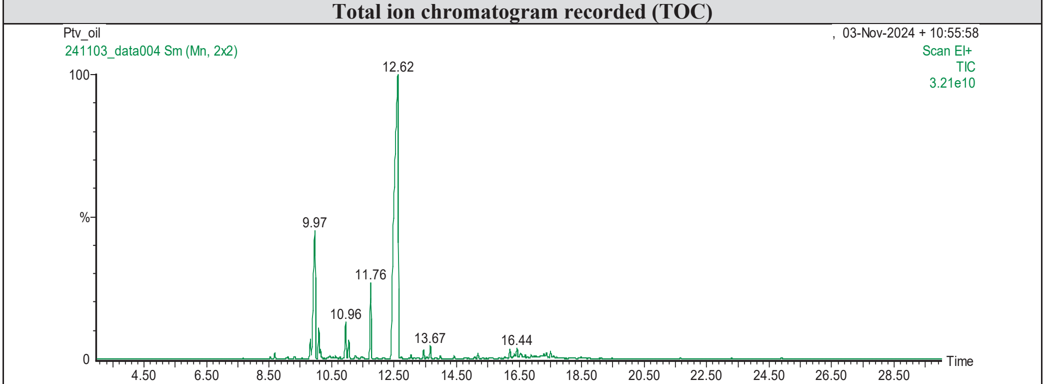
Other compounds, such as 2,5,5-trimethyl-3,6-heptadien-2-ol (3.66%) and 1,5-heptadien-4-ol, 3,3,6-trimethyl- (3.29%), while present in smaller quantities, add complexity to the overall chemical profile, possibly contributing to the scent or synergistic biological effects of the hydrosol.

For *Tanacetum vulgare* L. *essential oil*, the analyses indicate that the compound linalool oxide is the most abundant in the sample, accounting for 68.61% of the total area (Table 3, Figure 3).

Table 3. *Tanacetum vulgare* L. essential oil compounds

	Compound name	Retention time (min)	Probability (%)	CAS #	Area	% from the sum of areas
1	p-Cymene	8.55	93	99-87-6	8973151	0.13
2	1,8-Cineole	8.69	88.8	470-82-6	24311886	0.36
3	ç-Terpinene	9.10	90.9	99-85-4	7410893	0.11
4	Linalool	9.83	88.6	78-70-6	83461944	1.22
5	BICYCLO[3.1.0]HEXAN-3-ONE, 4-METHYL-1-(1-METHYLETHYL)-	9.95	98	1125-12-8	1071773248	15.72
6	á-THUJONE	10.10	90.9	471-15-8	128314760	1.88
7	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S-endo)-	10.96	89.3	464-45-9	186864848	2.74
8	Bicyclo[3.1.1]hept-2-en-6-ol, 2,7,7-trimethyl-, acetate, [1S-(1à,5à,6á)]-	11.77	71.8	50764-55-1	379507232	5.57
9	LINALOOL OXIDE	12.64	66.4	5989-33-3	4677715968	68.61
10	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl- (CAS)	15.09	88.2	644-30-4	7365104	0.11
11	GERMACRENE-D	15.19	86.5	23986-74-5	23497632	0.34
12	2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalen-2-yl)-prop-2-en-1-ol	16.05	75.5	-	10966000	0.16
13	GERANYL PENTANOATE	16.21	86.7	-	36780804	0.54
14	Caryophyllene oxide	16.44	85.9	1139-30-6	50738384	0.74
15	salvial-4(14)-en-1-one	16.54	79.1	-	20121556	0.30
16	trans-Sesquisabinene hydrate	16.70	84.1	145512-84-1	14278482	0.21
17	Neointermedeol	17.29	82.8	5945-72-2	10663753	0.16
18	á-Guaiene	17.38	82	88-84-6	19988978	0.29
19	(R)-1-Methyl-4-(6-methylhept-5-en-2-yl)cyclohexa-1,4-diene	17.51	83.4	28976-67-2	32698910	0.48
20	Lanceol, cis	17.71	75.2	10067-28-4	3732649	0.05
21	Spiro[4.5]decan-7-one, 1,8-dimethyl-8,9-epoxy-4-isopropyl-	18.49	73.8	61050-91-7	6015779	0.09
22	Phytol	21.66	85.9	150-86-7	5517628	0.08
23	Tricosane (CAS)	23.30	89.3	638-67-5	2018076	0.03
24	Tetracosane	24.90	87.7	646-31-1	3690392	0.05
25	Pentatriacontane (CAS)	26.38	84.7	630-07-9	1259301	0.02

Total ion chromatogram recorded (TOC)



**Ptv oil - Tanacetum vulgare* L. essential oil compounds

Figure 3. *Tanacetum vulgare* L. essential oil TOC

This compound is highly prevalent and likely contributes significantly to the aroma and therapeutic properties of the oil, given its common use in fragrances and as a bioactive compound. Several terpenes are present, including α-thujone (1.88%), bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)- (15.72%), and bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl- (2.74%).

These compounds contribute to the essential oil's fragrance profile and may have various biological effects, such as antimicrobial or calming properties. Other compounds such as geranyl pentanoate (0.54%), caryophyllene oxide (0.74%), and germacrene-D (0.34%) are present in lower quantities but still add to the complexity of the chemical profile. These compounds are often linked to earthy or spicy aromas and could contribute to the oil's overall effects.

Compounds such as p-cymene, 1,8-cineole, and geranyl pentanoate suggest a potential for aromatic, citrus-like, or herbal scents, which are common in essential oils used in perfumery, aromatherapy, and other applications.

In a 2004 study, it is mentioned that four chemotypes of *Tanacetum* were identified in Lithuania, each with different major components (Mockute D., 2004):

Chemotype 1: camphor and 1,8-cineole;
Chemotype 2: á-thujone and 1,8-cineole;
Chemotype 3 : 1,8-cineole;
Chemotype 4: artemisia ketone and camphor .

The analyzed sample is part of chemotype 2.

The analyses of *Tanacetum* hydrosol revealed its distinctive chemical composition (Table 4, Figure 4). The compound 2H-Pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-, acetate, trans- is the most abundant in the sample, comprising 89.76% of the total area. This suggests that it plays a significant role in the overall chemical composition and likely contributes the most to the hydrodol's or fragrance and potential biological effects.

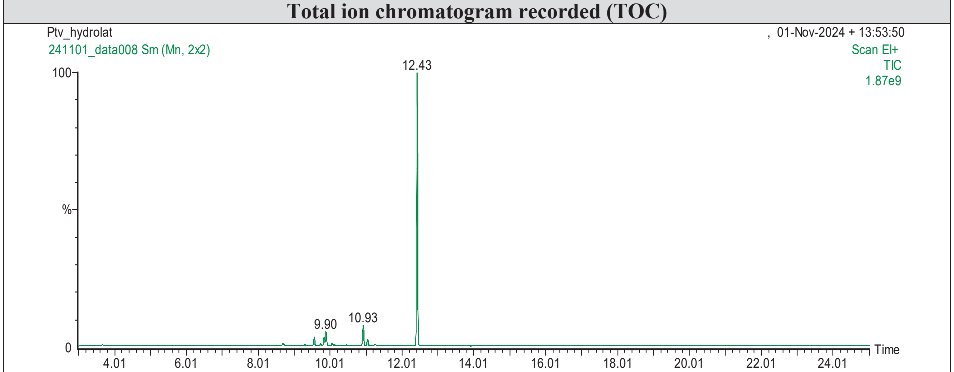
Other important compounds like thujone (4.33%) and trans-linalool oxide (3.24%) are also present, indicating the presence of bioactive terpenes known for their aromatic and therapeutic properties. Thujone, in particular, is known for its neurotoxic and medicinal effects in small doses, while linalool oxide is linked to calming and antimicrobial properties.

The compound 2H-Pyran-3(4H)-one, 6-ethenyldihydro-2,2,6-trimethyl- (2.67%) contributes to the complexity of the hydrosol's or overall profile, likely adding to the fragrance and biological activity.

Table 4. *Tanacetum vulgare* L. hydrolat compounds

	Compound name	Retention time (min)	Probability (%)	CAS #	Area	% from the sum of areas
1	trans-Linalool oxide	9.56	89.4	34995-77-2	2448745	3.24
2	2H-Pyran-3(4H)-one, 6-ethenyldihydro-2,2,6-trimethyl-	9.84	87.6	33933-72-1	2022886	2.67
3	Thujone	9.90	89.5	546-80-5	3274052	4.33
4	2H-Pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-, acetate, trans-	12.43	88.9	56752-50-2	67910624	89.76

Total ion chromatogram recorded (TOC)



*Ptv hydrosol – Plant *Tanacetum vulgare* L. hydrosol

Figure 4. *Tanacetum vulgare* L. hydrolat TOC

CONCLUSIONS

The *Santolina chamaecyparissus* L.essential oil is characterized by a complex blend of terpenes, sesquiterpenes, and oxygenated compounds, with longiverbenone being the most abundant. This diverse composition suggests that the oil may have both aromatic and therapeutic applications, with the potential for use in the fragrance industry as well as for its bioactive properties, including antimicrobial, anti-inflammatory, and antioxidant effects. The high percentage of terpene compounds further underscores the potential commercial value of the oil.

The *Santolina chamaecyparissus* L. hydrosol appears to have a diverse and potentially beneficial composition, with longiverbenone being the most abundant compound, likely contributing significantly to its aroma and bioactivity. The high concentration of other terpenes and oxygenated compounds further supports its potential in various commercial and therapeutic applications.

The *Tanacetum vulgare* L. essential oil sample, with linalool oxide (68.61%), key terpenes like α-thujone (1.88%) and diverse minor compounds, shows potential for applications in perfumery, therapeutics, and personal care due to its complex aromatic and bioactive properties.

The *Tanacetum vulgare* L. hydrolat sample's composition, dominated by 2H-Pyran-3-ol acetate (89.76%) and supported by bioactive compounds like thujone and trans-linalool oxide, indicates strong potential for applications in perfumery, therapeutics, and antimicrobial products.

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