

Essential oil profile of yarrow (*Achillea* spp. and *Tanacetum* spp.) ecotypes and their allelopathic potential to suppress redroot pigweed (*Amaranthus retroflexus* L.)

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Abstract

As far as we know, there is no information on the effect of *Achillea* residuals on controlling weeds when considering the effective compounds of the aerial parts of this plant. Thus, in a pot experiment, the allelopathic effect of dry material from the flower, leaf and stem of *Tanacetum polycephalum* L. and 9 *Achillea* spp. (*Achillea santolina* L., *A. millefolium* L., *A. nobilis* L., *A. conferta* DC., *A. vermicularis* Trin., *A. beibersteinii* Afan., *A. talagonica* Boiss., *A. tenuifolia* Lam., *A. aleppica* DC.) applied to the soil on the growth of redroot pigweed (*Amaranthus retroflexus* L.) seedling was tested. Five different ratios of aerial dry material of different species as residues (at 0, 10, 20, 40, and 50 g kg⁻¹ dry weight) were used in the pots. *Achillea* residual had a significant effect on the growth of redroot pigweed. *Achillea vermicularis*, *A.conferta*, *A. aleppica*, and *A. nobilis* were the most effective species at stopping the growth of redroot pigweed. Based on the results of GC/MS analyses, 152 different compounds were found in the essential oil of *Achillea* spp. Partial least squares regression between effective doses for controlling redroot pigweed and allelochemical compounds of *Achillea* species showed that cis-Menth-2-en-1-ol, α -Terpinyl, propionate and Bornyl acetate had the most effect on inhibiting the growth of redroot pigweed. Our research revealed that the *Achillea* genus has a lot of potential as a bioherbicide. This means that its leftovers or mulch could be used as a good cover crop to get rid of redroot pigweed.

Introduction

Weed control on farms is becoming harder because costs are going up and weeds are becoming resistant to herbicides. More than 5 percent of all the biotypes of the 180 different species of weeds that have become resistant to herbicides come from the *Amaranthus* genus¹. They have evolved resistance to diverse herbicides like those that inhibit photosystem II (PS II), acetolactate synthase (ALS), protoporphyrinogen oxidase (PPO), and 5-enolpyruvyl-shikimate-3-phosphate synthase (EPSPS)^{2,3}. Agrochemicals (fertilizers and pesticides) used in conventional agriculture pose health and environmental risks.

Allelopathy has been defined as the suppression of growth of one plant species by another through the release of toxic substances (known as allelochemicals) into the environment⁴, which includes the inhibitory effects of one plant species on another one. According to Dragoeva et al.⁵, allelopathy could become one of the key sciences that help protect the environment and boost agricultural production. So, allelopathic compounds could be considered an alternative to synthetic agrochemicals.

The genus *Achillea* (Asteraceae) has roughly 130–140 perennial herb species, the majority of which are found in Eurasia, some in North Africa, and a few in North America and the Southern Hemisphere^{6,7,8,9,10}. This genus contains around 19 indigenous species in Iran^{11,12,13}. The *Achillea* genus is a medicinal plant whose therapeutic applications have been widely reported^{14,15}. Flavonoids, phenolic acids, coumarins, lignans, amino acid derivatives, fatty acids, terpenoids, alkalamides, and sterols are among the phytochemicals found in *Achillea* species. Some of these compounds, such as terpenoids, flavonoids,

phenolic acids, and coumarins, exhibit allelopathic effects^{16,17,18}. Because of this, *Achillea* can be seen as a good source of chemicals, and recent authors have stated this in their work^{19,20}. For instance, aqueous extracts of yarrow (*Achillea millefolium* L.) inhibited the germination and growth of redroot pigweed²⁰. The allelopathic potential of *Achillea santolina* aqueous extract and plant residuals was evaluated in pea (*Pisum sativum*), wheat (*Triticum aestivum* L.), safflower (*Carthamus tinctorius*), faba bean (*Vicia faba* L.), and barley (*Hordeum vulgare*)^{22,23}. A bioassay with lettuce (*Lactuca sativa* L.) seed revealed that several *Achillea* inhibited growth, with *Achillea wilhelmsii* and *Achillea filipendula* inflorescences showing the largest (96%) decrease. Furthermore, radicle elongation was suppressed (by 83–95%) in lettuce that had been treated with extracts from *Achillea nobilis* flower and *Achillea biebersteinii* leaf¹⁹. *Amaranthus retroflexus* had less germination, a lower germination rate, smaller seedlings, and shorter roots when essential oils from *Achillea* spp. were used²⁴.

One study found that the main oil constituents of 42 *Achillea* species in Turkey were santolina alcohol, 1,8-cineole, cis-chrysanthenyl acetate, linalool, spathulenol, terpinen-4-ol, α -terpineol, β -eudesmol, artemisia ketone, p-cymene, camphor, caryophyllene oxide, α -pinene, linalool, trans-pinocarveol, and trans-verbenol²⁵. These compounds belong to the classes phenolics, terpenoids, and terpenes, which can cause strong allelopathic effects.

As far as we are aware, there is no evidence on the influence of *Achillea* residuals on weed control when considering the active chemicals of this plant's aerial parts. So, the purpose of this experiment was to see how different residual amounts of *Achillea* species left in the soil affected the growth and emergence of redroot pigweed seedlings.

Result And Discussion

Essential oil yield

From the aerial biomass of *Achillea* and *Tanacetum* species, the essential oil yield ranged from 0.024–1.732% (Table 1). In this case, it's also important to address how differences in physiology, environment, geography, genetics, and evolution affect the content of essential oils and chemical composition of different species^{26,27}.

Table 1
essential oil yield of species

Species	Essential oil content (%)
<i>Achillea aleppica</i>	0.482
<i>Achillea teonifolia</i>	-
<i>Tanacetum polycephalum</i>	0.115
<i>Achillea teonifolia</i>	0.15
<i>Achillea teonifolia</i>	0.0532
<i>Achillea vermicularis</i>	0.024
<i>Achillea biebersteinii</i>	0.262
<i>Achillea talagonica</i>	0.236
<i>Achillea santolina</i>	0.482
<i>T. polycephalum</i>	1.732
<i>Achillea bibrestini</i>	0.08
<i>Achillea teonifolia</i>	0.039
<i>Achillea milifolium</i>	0.051
<i>Achillea pachycephala</i>	0.029
<i>Achillea nobilis</i>	0.158
<i>Achillea conferta</i>	0.148

Allelopathic effects on redroot pigweed seedling growth

The four-parameter log-logistic model's results show how much the dry matter of *Achillea* species could cause the dry matter of redroot pigweed to go down by 10, 50, and 90% (Table 2). All species had a significant influence on redroot pigweed seedling growth. According to Table 2, 0.02, 10.00, 2.12, 10.26, 0.07, 9.01, 4.97, 6.70, 10.35, 6.70, 10.35, 9.20, 10.00, and 9.00 g dry matter of *A. alppica* from Ilam, *A. teonifolia* from Markazi, *T. polycephalum* from Lorestan, *A. teonifolia* from Hamedan, *A. vermicularis* from Mazandaran, *A. pachycephala* from Lorestan, *A. talagonica* from Markazi, *T. polycephalum* from Mazandaran, *A. teonifolia* from Tehran, *A. milifolium* from Hamedan, *A. nobilis* from Lorestan, and *A. conferta* from Ilam, each respectively per 1 kg soil, reduced the dry matter of redroot pigweed by 90%. In practice, if the weight of one hectare of soil is assumed to be around 3000 tons, depending on species, it will take between 60 and 31000 kg of yarrow dry matter per hectare to control 90% of redroot pigweed.

Table 2

The obtained parameters come from the four-parameter log-logistic model. In this model, the dry weight of the redroot pigweed's aboveground parts was a response variable, and the different rates of the dry residue of *Achillea* species were independent variables. *b*, *min*, *max*, *ED*₁₀, *ED*₅₀, and *ED*₉₀ are the slope, upper bound, lower bound, and effective rates for controlling redroot pigweed at 10, 50, and 90%, respectively. The species denoted with a * have the greatest allelopathic effect on redroot pigweed seedling growth. The values in arenteses are standard errors.

Species	<i>b</i>	<i>min</i> (%)	<i>max</i> (%)	<i>ED</i> ₁₀	<i>ED</i> ₅₀ g kg ⁻¹	<i>ED</i> ₉₀	R ²	RMSE
<i>Achillea aleppica</i> *	0.179 (3.08)	0.00	100 (12.50)	0.01 (0.001)	0.01 (0.001)	0.02 (0.01)	0.84	21.66
<i>Achillea teonifolia</i>	1.00 (0.38)	1.00 (0.90)	100 (22.38)	1.0 (0.90)	4.1 (2.99)	10.00 (9.02)	0.41	38.76
<i>T. polycephalum</i>	1.23 (0.65)	0.00	99.99 (12.57)	0.31 (0.25)	1.88 (0.78)	2.12 (1.03)	0.84	21.78
<i>Achillea teonifolia</i>	1.00 (0.95)	10.0 (9.0)	100 (20.21)	5.77 (4.40)	10.0 (9.01)	10.26 (9.40)	0.50	35.01
<i>Achillea vermicolaris</i> *	0.15 (0.07)	0.00	99.99 (17.73)	0.01 (0.001)	0.058 (0.04)	0.070 (0.05)	0.77	30.7
<i>A. pachycephala</i> *	13.99 (5.4)	3.64 (1.33)	100 (13.20)	0.002 (0.001)	8.29 (7.00)	9.01 (8.00)	0.79	22.86
<i>Achillea talagonica</i> *	0.75 (0.59)	0.00	100 (12.47)	0.67 (0.50)	1.11 (0.70)	4.97 (3.73)	0.84	21.61
<i>T. polycephalum</i>	1.06 (0.797)	0.00	99.83 (14.13)	0.74 (0.07)	5.9 (5.22)	6.70 (4.36)	0.83	24.47
<i>Achillea teonifolia</i>	6.083 (3.19)	16.00 (10.00)	99.93 (15.82)	7.4 (6.22)	9.64 (7.45)	10.35 (8.05)	0.77	27.43
<i>Achillea milifolium</i>	13.88 (4.75)	11.45 (8.63)	99.99 (13.61)	4.144 (0.05)	5.930 (4.90)	9.2 (8.21)	0.76	23.58
<i>Achillea nobilis</i>	1.00 (0.45)	1.00 (0.60)	10.0 (9.00)	1.93 (0.05)	8.00 (6.04)	10.00 (9.03)	0.39	39.44

Species	<i>b</i>	<i>min</i>	<i>max</i>	<i>ED</i> ₁₀	<i>ED</i> ₅₀	<i>ED</i> ₉₀	R ²	RMSE
		(%)	(%)		g kg ⁻¹			
<i>Achillea conferta</i> *	1.00	1.00	100	0.01	7.00	9.0	0.41	38.78
	(0.4)	(0.50)	(22.39)	(0.001)	(4.02)	(7.06)		

Essential oil composition

More than 152 compounds were found in different amounts in the essential oils of 13 species of yarrow. The main goal of this research was to focus on the five species that stopped redroot pigweed from growing the most. Based on the values of the parameters in the PLS regression model, α -Pinene, camphene, β -Pinene, 2,3-Dehydro-1,8-cineole, Yomogi alcohol, α -Phellandrene, α -Terpinen, p-Cymene, 1,8-Cineole, τ -Terpinen, Terpineol, cis- β , α -Thujone, p-Menth-2-en-1-ol, Camphor, Pinocarvone, Borneol, Terpinen-4-ol, p-Cymen-8-ol, α -Terpieol, trans-Piperitol, Carveol < trans->, Piperitone, Bornyl acetate, Thymol, Carvacrol, α -Copaene, Jasmone, Caryophyllene, β -Cubebene, Aromadendrene oxide-(2), (-)-Spathulenol, Caryophyllene oxide, β -Eudesmol, palmitic acid, and linolenic acid were found to be the most important parts of the species' essential oil (Tables 4 and 5). Piperitone followed by camphor, 1,8-Cineole, α -Terpieol, Borneol, Spathulenol, Terpinen-4-ol, and palmitic acid, were the most common components of essential oils, and different species had different amounts of them (Table 3). Even though a large proportion of Piperitone was identified in the essential oils of *Achillea* and *Tanacetum* spp., our results showed that this compound doesn't have a strong allelopathic effect on the growth of pigweed redroot seedlings. There are no clear evidences in literatures about allelopathic effect of Piperitone²⁸. Camphor has been shown in some studies to act as an allelochemical^{29,30}. In one study, 1,8-cineole suppressed the seedling growth and fresh weight of lettuce (*Lactuca sativa*)³¹. In one germination experiment, α -terpineol inhibited the growth of redroot pigweed³². Terpenes such as borneol have an allelopathic effect on other plants^{29,33}. Researchers showed that Spathulenol was the most active of the allelochemicals that can inhibit plant growth³⁴. Furthermore, several terpenes, like β -caryophyllene, δ -terpinene, and α -pinene, inhibited the growth of some plants³⁵. The four volatile compounds that contribute the most to star anise's volatile allelopathy were L-fenchone, 1,8-cineole, β -pinene, and camphene³⁶. Pinene is a monoterpene well known for its phytotoxic action, but little is known about the allelopathic effect of its isomers. For example, α -pinene strongly inhibited mitochondrial ATP production in plants³⁷. In a study, on the other hand, α -pinene made the target plant grow faster while β -pinene slowed it down³⁸. The allelopathic effects of other minor components are also mentioned in some articles. Linhart³⁹ found that monoterpenes (geraniol, α -terpineol, cis-sabinene hydrate, linalool, or 1,8-cineole) or phenolic compounds (carvacrol and thymol) made by common thyme (*Thymus vulgaris*) can stop *Daucus carota*, *Nigella damascena*, and *Bromus madritensis* from germinating, establishing themselves, and/or growing. Table 3 shows all chemicals from the five *Achillea* species, except those with trace levels. We used the

log-logistic and PLS models to find the most effective compounds, and we think that allelochemicals can have an antagonistic and antithetical effect. Conversely, some components have a stimulatory effect on the growth of redroot pigweed seedlings (Table 5). The most important compounds identified with the models were germacrene-D, bicyclogermacrene, camphor, borneol, 1,8- cineole, α -Thujone, bornyl acetate, Borneol, 1,8-cineole, τ -Terpinen, Terpineol, cis- β , α -Terpieol, p-Menth-2-en-1-ol, Camphor, Borneol, Terpinen-4-ol, α -Terpieol, trans-Piperitol, Piperitone, Bornyl acetate, (-)-Spathulenol, β -Eudesmol, and palmetic acid. Fatty acids are found in the essential oil because the aerial parts (inflorescence with seeds) were ground up.

Identification of the compounds with GC-MS analyses and comparison with bioassays yielded significant findings (Tables 3–5). The amount of yarrow residue that was expected at three levels (ED10, ED50, and ED90) was plotted against the amount that was actually found (Fig. 1). As can be seen in ED50, the difference between what was predicted and what was measured is getting smaller. The smaller the gap between the blue line and the dashed line, the more precise the measurements will be (Fig. 1). The purpose of this experiment is to identify compounds for further experiments. We can do these experiments with pure essential oil compounds, and it is necessary to perform this test in the future.

Table 3

The essential oil components identified in the strongest allelopathic species. The reporting of very detailed compounds has been omitted.

RI	Compound	Essential oils components (%)				
		<i>A. aleppica</i>	<i>A. vermicolaris</i>	<i>A. biebersteinii</i>	<i>A. talagonica</i>	<i>A.conferta</i>
950	α -Pinene	0.48	0.05	0.09	0.05	0.02
965	Camphene	0.21	0.02	0.1	0.04	0.01
991	Sabinene					0.08
995	β -Pinene	0.1			0.05	0.02
1007	2,3-Dehydro-1,8-cineole	0.11	0.02	0.02	0.05	0.04
1014	Yomogi alcohol		0.02			
1021	α -Phellandrene		0.07	0.13	0.2	
1032	α -Terpinen		0.05	0.06	0.1	0.06
1039	p-Cymene	1.42		0.6		
1039	β -Cymene		0.2			0.29
1039	o-Cymene				0.51	
1043	Limonene	0.49				
1048	1,8-Cineole	0.38	2.9	6.89	5.76	4.95
1073	τ -Terpinen	0.19	0.17	0.09	0.07	0.31
1083	Sabinene hydrate			0.29		1.55
1115	Terpineol, cis- β -		0.73	0.5	0.55	1.88
1122	α -Thujone			0.85		2.93
1133	β -Thujone					3.97
1140	cis-Menth-2-en-1-ol			4.69		
1161	p-Menth-2-en-1-ol			5.33	5.7	0.39
1141	Chrysanthenone	0	2.79			0.56
1157	cis-Sabinol					1.44
1161	Camphor	2.97	11.43	9.28	3.65	2.45
1181	Pinocarvone		0.38	0.24	0.22	

RI	Compound	Essential oils components (%)				
1184	Borneol	0.41	2.23	1.13	0.79	1.84
1194	Terpinen-4-ol	0.95	2.31	0.86	0.61	3.66
1203	Cryptone	0.18		0.27	0.43	
1202	p-Cymen-8-ol		0.11			
1209	α -Terpieol	3.16		1.48	1.08	3.55
1213	cis-Piperitol			1.62	1.85	
1214	Fir Balsam Canada 20% RT12.582 SC937 RI1204 PR83 FG99		1.08			
1213	Myrtenol					0.31
1228	trans-Piperitol		0.54	3.32	3.92	
1237	Carveol < trans->		0.49	0.24	0.12	
1278	Chrysanthenyl acetate < trans					2.05
1285	Piperitone	79.9	3.85	34.1	45.92	1.65
1295	Phellandral				0.31	
1304	Bornyl acetate		0.56	2.92	1.08	1.42
1308	Sabinyll acetate < trans->					0.41
1310	p-Cymen-7-ol			0.54	0.55	
1315	Terpinene 4-acetate					0.33
1322	Thymol		0.9	0.32	0.39	
1323	Tea-tree-EB-10pcent					
1330	Carvacrol	0.59	0.47	0.32	0.18	
1353	Carvyl acetate < trans>		0.23			
1393	α -Copaene		0.17			
1409	Decanoic acid			0.6	0.28	0.62
1409	β -Elemene					0.73
1412	3,5-Heptadienal, 2-ethylidene-6-methyl-		2.69			

RI	Compound	Essential oils components (%)		
1414	Yarrow-blue-EB- 10pcent RT17.709 SC1438 RI1398 PR78 FG90	1.22		
1417	Jasmone		0.27	
1422	Methyleugenol	0.8		2.17
1438	Caryophyllene		0.07	0.1
1473	β -Farnesene			0.42

1494	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7					0.98
1501	τ -cadinene					1.93
1501	β -Cubebene				0.35	
1501	Germacrene D		0.36			
1506	Selinene < beta					1.94
1505	β -Ionone		0.92			
1516	Bicyclogermacrene					0.5
1543	δ -Cadinene		0.25			
1561	α -Terpinyl propionate			0.53		
1582	Nerolidol		0.43	0.12	0.48	13.44
1589	Aromadendrene oxide-(2)		0.78	0.16	0.11	
1606	(-)-Spathulenol		2.87	0.64	0.46	3.03
1604	Caryophyllene oxide	0.37	0.67	0.28	0.31	
1617	Aristolene epoxide		0.89			
1617	Fokienol					2.02
1818	Aristolene epoxide		0.89			
1642	4-(4-Methylphenyl) pyridine		0.63			
1648	Unknown					1.4
1654	γ -Eudesmol					1.57
1673	β -Eudesmol		1.12		0.48	5.35
1710	Artemisia 7 04-06-12 20% RT23.558 SC2009 RI1625 PR86 FG98					2.06
1995	Palmitic acid		5.03		2.13	1.49
2168	Linolenic acid		1.64		0.72	
2169	Linolenic acid, methyl ester					1.31

Table 4 displays the positive and negative coefficients for the amount to which each component has inhibitory or stimulatory effects on redroot pigweed seedlings. However, certain compounds have different effects on various EDs. Yomogi alcohol, for example, decreases (inhibits) all EDs, but cis-Menth-2-en-1-ol inhibits ED10 while stimulating the development of ED50 and ED90. So, it makes sense to think

that the most important allopathic inhibitors that can be extracted and studied are those with negative coefficients within each ED. Furthermore, EDs that are affected by both positive and negative effects show that allopathic substances have both positive and negative allelochemical effects, which should be looked into more in the future. Another important fact is that the action of allelochemicals changes when they are mixed with other allelochemicals, and when an allopathic substance is mixed with other substances, the effects of each substance overlap and either get stronger or weaker. Table 4 further revealed that compounds such as α -Pinene, Yomogi alcohol, Limonene, Chrysanthenone, p-Cymen-8-ol, Fir Balsam Canada 20% RT12.582 SC937 RI1204 PR83 FG99, Carvacrol, Carvyl acetate < trans>, α -Copaene; 3,5-Heptadienal, 2-ethylidene-6-methyl, Yarrow-blue-EB-10pcent RT17.709 SC1438 RI1398 PR78 FG90, Germacrene D, β -Ionone, δ -Cadinene, Aromadendrene oxide-(2), Caryophyllene oxide, Aristolene epoxide, Aristolene epoxide, and 4-(4-Methylphenyl)pyridine had unfavorable impacts on redroot pigweed whereas Terpineol cis- β -, p-Menth-2-en-1-ol, cis-Piperitol, and trans-Piperitol have good effects at all three EDs. In different experiments, it was shown that the phytotoxic activity of leaf powder and (+)-camphor in soil was related to the concentration of (+)-camphor in soil water. It was thought that the allelopathic activity of (+)-camphor in soil treated with the leaf powder was mostly caused by (+)-camphor released from the leaf powder into the soil and (+)-camphor taken in from the air through the stomata⁴. Terpinen-4-ol is a chemical compound with the strongest antimicrobial and antibacterial activity. It can stop lettuce from sprouting and growing roots and shoots⁴⁰. 1,8-cineole is also an antifungal compound with allelopathic action in soil^{4,41}. Allelopathic effects have been attributed to borneol, 1,8-cineole, camphor, and piperitone in several investigations^{42,43}. We look for individual compounds, but many of these compounds and their interaction in allelopathy are unknown.

Table 5 shows the biological activity of each allelochemical at the three EDs. The compounds with larger coefficients indicate that the allelopathic material has a bigger effect, while those with coefficients equal to zero indicate that the substance has no influence on the allelopathic process. According to our results with the model between the dry matter of redroot pigweed and the components of essential oils, for example, Decanoic acid and cis-Menth-2-en-1-ol. have been identified as two important compounds in yarrow allelopathy, along with Santolina triene and Pinocarvone, which had no influence on the allelopathic process. The most effective essential elements include cis-Menth-2-en-1-ol, α -Terpinyl, propionate, Bornyl acetate, o-Cymene, Phellandral, Jasmone, β -Cubebene, Decanoic acid, 1,8-Cineole, α -Thujone, and Carvacrol (Table 5). Our results were consistent with previous studies. Some literature has reported that some long-chain fatty acids have an allelopathic effect and are natural phytotoxins. According to bioassays, nonanoic and decanoic acids have phytotoxic effects on algae^{4,44}

Tables 4 and 5 also show that these allelopathic compounds can be found in many different plants, extracted, and used to make bioherbicides. Future experiments on allelopathy will have to focus on the production and bioassay of pure components and combine them in separate experiments. Limonene, for example, can be extracted from the citrus⁴⁵, jasmone from jasmine flowers⁴⁶, camphene and bornyl acetate from *Valerianaceae* spp.⁴⁷, α -Thujone from *Artemisia absinthium* L., and other important compounds from species with most of these allelochemicals.

Table 4

Standard coefficients of each of the essential oil components in relation to effective doses (ED)

Compounds	(ED10)	(ED50)	(ED90)
camphene	-0.033	0.005	-0.008
β -Pinene	0.05	-0.061	-0.047
2,3-Dehydro-1,8-cineole	0.031	-0.05	-0.043
Yomogi alcohol	-0.014	-0.019	-0.027
α -Phellandrene	0.052	-0.012	0.011
α -Terpinen	0.062	-0.011	0.016
β -Cymene	-0.012	0.004	-0.002
o-Cymene	0.111	-0.067	-0.026
Limonene	-0.007	-0.027	-0.034
1,8-Cineole	-0.003	0.051	0.057
τ -Terpinen	-0.022	0.005	-0.007
Sabinene hydrate	-0.02	0.036	0.03
Terpineol, cis- β -	0.001	0.019	0.02
α -Thujone	-0.029	0.047	0.038
β -Thujone	-0.003	0.018	0.016
cis-Menth-2-en-1-ol	-0.086	0.095	0.071
p-Menth-2-en-1-ol	0.026	0.02	0.036
cis-Sabinol	-0.003	0.018	0.016
Camphor	-0.064	0.043	0.021
Pinocarvone	-0.004	0.003	0.003
Borneol	-0.03	0.021	0.009
Terpinen-4-ol	-0.02	0.013	0.003
Cryptone	0.056	-0.02	0.004
α -Terpieol	-0.013	0.014	0.008
cis-Piperitol	0.031	0.014	0.031
Myrtenol	-0.003	0.018	0.016
trans-Piperitol	0.033	0.01	0.028

Compounds	(<i>ED</i> 10)	(<i>ED</i> 50)	(<i>ED</i> 90)
Carveol < trans->	-0.031	0.013	0.001
Chrysanthenyl acetate < trans	-0.003	0.018	0.016
Piperitone	0.021	-0.028	-0.022
Phellandral	0.111	-0.067	-0.026
Bornyl acetate	-0.059	0.089	0.076
Sabinyll acetate < trans->	-0.003	0.018	0.016
p-Cymen-7-ol	0.021	0.022	0.036
Terpinene 4-acetate	-0.003	0.018	0.016
Thymol	0.004	-0.015	-0.014
Decanoic acid	-0.033	0.072	0.066
β -Elemene	-0.003	0.018	0.016
Jasmone	0.111	-0.067	-0.026
Methyleugenol	-0.009	0.011	0.006
Caryophyllene	0.047	-0.001	0.022
β -Farnesene	-0.003	0.018	0.016
2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7	-0.003	0.018	0.016
X59 τ -cadinene	-0.003	0.018	0.016
β -Cubebene	0.111	-0.067	-0.026
Selinene < beta	-0.003	0.018	0.016
Bicyclogermacrene	-0.003	0.018	0.016
δ -Cadinene	-0.014	-0.019	-0.027
α -Terpinyl propionate	-0.086	0.095	0.071
Nerolidol	-0.001	0.016	0.015
Aromadendrene oxide-(2)	-0.017	-0.009	-0.017
(-)-Spathulenol	-0.017	0.009	0.002
Fokienol	-0.003	0.018	0.016
unknown	-0.003	0.018	0.016
γ -Eudesmol	-0.003	0.018	0.016

Compounds	(<i>ED</i> 10)	(<i>ED</i> 50)	(<i>ED</i> 90)
Artemisia 7 04-06-12 20% RT23.558 SC2009 RI1625 PR86 FG98	-0.003	0.018	0.016
Palmitic acid	0.035	-0.046	-0.036
Linolenic acid	0.035	-0.049	-0.039
Linolenic acid, methyl ester	-0.003	0.018	0.016

Table 5
Importance of allelochemicals for each effective dose (ED).

compound	ED10	ED50	ED90
cis-Menth-2-en-1-ol	1.024	0.830	1.726
α -Terpinyl propionate	1.024	0.830	1.726
Bornyl acetate	1.529	1.272	1.665
o-Cymene	0.552	1.422	1.553
Phellandral	0.552	1.422	1.553
Jasmone	0.552	1.422	1.553
β -Cubebene	0.552	1.422	1.553
Decanoic acid	1.876	1.549	1.520
1,8-Cineole	1.301	1.327	1.315
α -Thujone	1.673	1.379	1.216
Carvacrol	1.389	1.302	1.189
Sabinene hydrate	1.562	1.290	1.135
p-Menth-2-en-1-ol	0.428	1.170	1.120
α -Terpinen	0.511	1.236	1.120
Caryophyllene oxide	1.528	1.265	1.113
p-Cymen-7-ol	0.374	1.122	1.107
Caryophyllene	0.154	1.245	1.105
cis-Piperitol	0.299	1.166	1.096
trans-Piperitol	0.176	1.154	1.077
β -Pinene	0.966	0.784	1.074
α -Phellandrene	0.207	1.202	1.059
Camphor	0.237	0.423	1.052
sabinene	1.324	1.098	1.027
β -Thujone	1.324	1.098	1.027
cis-Sabinol	1.324	1.098	1.027
Myrtenol	1.324	1.098	1.027
Chrysanthenyl acetate < trans	1.324	1.098	1.027

compound	ED10	ED50	ED90
Sabinyl acetate < trans->	1.324	1.098	1.027
Terpinene 4-acetate	1.324	1.098	1.027
β -Elemene	1.324	1.098	1.027
β -Farnesene	1.324	1.098	1.027
2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7	1.324	1.098	1.027
τ -cadinene	1.324	1.098	1.027
Selinene < beta	1.324	1.098	1.027
Bicyclogermacrene	1.324	1.098	1.027
Fokienol	1.324	1.098	1.027
unknown	1.324	1.098	1.027
γ -Eudesmol	1.324	1.098	1.027
Artemisia 7 04-06-12 20% RT23.558 SC2009 RI1625 PR86 FG98	1.324	1.098	1.027
Linolenic acid, methyl ester	1.324	1.098	1.027
Nerolidol	1.309	1.080	1.022
Cryptone	0.299	1.162	1.021
Terpineol, cis- β -	1.312	1.064	0.973
β -Eudesmol	1.150	0.960	0.966
τ -Terpinen	0.660	0.986	0.958
Linolenic acid	1.154	0.939	0.943
2,3-Dehydro-1,8-cineole	0.859	0.720	0.933
Methyleugenol	1.018	0.932	0.902
Terpinen-4-ol	0.854	0.927	0.865
Limonene	0.900	0.925	0.849
Palmitic acid	0.803	0.650	0.819
α -Pinene	0.895	0.913	0.805
p-Cymen-8-ol	0.896	0.882	0.776
3,5-Heptadienal, 2-ethylidene-6-methyl-	0.896	0.882	0.776
Yomogi alcohol	0.896	0.882	0.776

compound	ED10	ED50	ED90
Fir Balsam Canada 20% RT12.582 SC937 RI1204 PR83 FG99	0.896	0.882	0.776
Carvyl acetate < trans>	0.896	0.882	0.776
α -Copaene	0.896	0.882	0.776
Yarrow-blue-EB-10pcent RT17.709 SC1438 RI1398 PR78 FG90	0.896	0.882	0.776
Germacrene D	0.896	0.882	0.776
β -Ionone	0.896	0.882	0.776
δ -Cadinene	0.896	0.882	0.776
Aristolene epoxide	0.896	0.882	0.776
Aristolene epoxide	0.896	0.882	0.776
4-(4-Methylphenyl)pyridine	0.896	0.882	0.776
β -Cymene	0.664	0.769	0.766
p-Cymene	0.475	0.710	0.753
α -Terpieol	0.839	0.777	0.715
Chrysanthenone	0.650	0.774	0.690
Carveol < trans->	0.567	0.503	0.690
campene	0.613	0.666	0.679
Aromadendrene oxide-(2)	0.817	0.745	0.672
Piperitone	0.878	0.732	0.656
Pinocarvone	0.585	0.541	0.634
(-)-spathulenol	0.574	0.674	0.623
Thymol	0.840	0.684	0.613
Borneol	0.473	0.599	0.539
Santolina triene	0.000	0.000	0.000
Pinocarvone	0.000	0.000	0.000

Figure 2 depicts the similarities and differences between the allelopathic species. The species were separated based on how much influence they had in different parts of the biplot. Species *Achillea aleppica* and *A. vermicolaris*, for example, are similar in composition and impact and are found in the same section.

In Fig. 3, two PLS components, t_1 and t_2 , and their correlation with allelochemicals and EDs are shown. Allelochemicals that have similar effective doses will be plotted closer together in the direction of that variable line (vector) and can be distinguished for efficacy. For instance, X50 (Decanoic acid) and X41 (Bornyl acetate) act the same, especially at ED_{90} (Fig. 3).

Conclusion

Our findings, based on the log-logistic model and PLS analysis, showed which chemicals play the most important role in yarrow allelopathy. The essential oil components of *Achillea* spp. as a suppressive plant for redroot pigweed control could be classified into three types: (1) inhibitory substances, (2) inhibitory and stimulatory substances, and (3) inert materials. So, it might be interesting to find new ways to make bioherbicides by isolating allelochemicals with inhibitory effects from different *Achillea* species. Also, looking at different combinations of them seems to show that the way they are put together is a key part of finding special compounds that inhibit or stimulate. *Achillea* species had a strong allelopathic effect on redroot pigweed. The essential oil components with the greatest inhibitory effect were cis-Menth-2-en-1-ol, α -Terpinyl, propionate and Bornyl acetate, in that order. Our research showed that the *Achillea* genus has a lot of potential as a bioherbicide. Because of this, the residues or mulch from these plants could be used as an effective cover crop to get rid of redroot pigweed. Five species, *A. vermicolaris*, *A. conferta*, *A. aleppica*, *A. biebersteinii*, and *A. nobilis*, more than other *Achillea* species, slowed down the growth of redroot pigweed.

Material And Methods

Plant materials

The aerial parts (flowers, leaves and stems) of the several *Achillea* and *Tanacetum* species were collected from the beginning of flowering to full bloom stages in eight provinces in Iran's north, west, south, and center. Based on the most recent research¹¹, these samples were found to be different species of *Achillea*. For each species, geographic coordinates and altitude are provided in (Table 6). Samples were taken to the lab of the Department of Agronomy at Tarbiat Modares University in Tehran, Iran, where they were dried at room temperature for two weeks. This comment should make it clear that there wasn't enough dry material for some species to be used in pot experiments.

Table 6
Achillea species collected from sixteen locations in eight provinces of Iran.

Species	Province	Location	Latitude	Longitude	Altitude
<i>Achillea aleppica</i>	Ilam	Anjireh	33.06 N	47.22 E	949
<i>Achillea teonifolia</i>	Markazi	Sarband	33.45 N	49.40 E	1958
<i>Tanacetum polycephalum</i>	Lorestan	Booryabaf	33.78 N	48.72 E	1617
<i>Achillea teonifolia</i>	Tehran	Tehran	35.32 N	51.17 E	941
<i>Achillea teonifolia</i>	Hamedan	Malayer	34.37 N	48.67E	1769
<i>Achillea vermicularis</i>	Mazandaran	Kandovan	36.14 N	51.30 E	2668
<i>Achillea biebersteinii</i>	Lorestan	Zereshgeh	33.86 N	48.70 E	1697
<i>Achillea talagonica</i>	Markazi	shazand	33.89 N	49.45 E	1974
<i>Achillea santolina</i>	Ilam	Anjireh	33.06 N	47.22 E	949
<i>T. polycephalum</i>	Mazandaran	Haraz	35.78 N	52.03 E	2651
<i>Achillea bibrestini</i>	Lorestan	Sheikhmiry	33.92 N	48.68 E	1694
<i>Achillea teonifolia</i>	Tehran	Vardavard	35.74 N	51.16 E	1279
<i>Achillea milifolium</i>	Hamedan	Hamedan	34.77 N	48.46 E	2157
<i>Achillea pachycephala</i>	Kermanshah	Bistoon	34.43 N	47.51 E	1299
<i>Achillea nobilis</i>	Lorestan	Zereshgeh	33.86 N	48.70 E	1697
<i>Achillea conferta</i>	Ilam	Kavar	32.97 N	46.84 E	941

Pot experiment

In the pot experiment, five different ratios of *Achillea* and *Tanactum* aerial parts (including flowers, leaves, and stems) residues (0, 10, 20, 40, and 50 g kg⁻¹ based on dry weight) were applied. The experiment was laid out in a completely randomized design with three replications. Plants were grown in plastic pots containing 1 kg of loamy sand soil. According to treatments, dry matter was mixed with 5 cm of soil surface layer, and then 10 redroot pigweed seeds were planted. The pots were placed in a greenhouse at a temperature of 25 to 30°C for three weeks. Then the fresh weight of seedlings was weighed immediately, and then the samples were dried in an oven at 70°C for 24 hours, and then their dry weight was measured with an analytical scale.

Essential oils extraction

Sample Preparation

Samples were air-dried in a dark room without sunlight, and then they were stored in a cool room (4°C) for subsequent experiments. All the aerial parts of each species were ground into a powder and put through a Clevenger type of hydro-distillation in order to get the essential oils. The best extraction process took 5 hours, used 350 watts of heat, and had a solid-to-solvent ratio of 1:10 g/mL at room temperature. The weight ratio of essential oil in dry materials was used to figure out the essential oil percentage. The water was taken out of the extracted essential oil by drying it over anhydrous sodium sulfate. The oil was then put in a sealed vial and kept at 4°C until it was time to test it again. The essential oil yield was calculated using the Eq. 1:

$$y = \frac{v \times 100}{w} \text{Eq.1}$$

where y is the essential oil yield (% v/w), V is the volume of collected essential oil (ml), and W is the weight of the plant material (g) (Table 1). Due to the low essential oil content in some species, the distillation method was performed several times, as indicated by Samadi et al⁴⁷.

GC/MS analysis

For the GC/MS analysis, a Hewlett-Packard 6890 gas chromatography system with a fused silica HP-5MS capillary column (30m x 0.25 mm x 0.25 pm) was used. The oven temperature was set to range from 60 to 280°C at 4°C/min. Helium was employed as a carrier gas at a flow rate of 2 ml/min. The chromatography was linked to a Hewlett-Packard 6890 mass-selective detector. The MS was set up to work with an ionization voltage of 70 eV and an ion source temperature of 200°C. The components of the oil were identified using retention indices relative to n-alkanes and computer matching with the main library, Replib, Adams, and Wiley 275.L, with NIST MS Search v. 2.0 and library, as well as by comparing fragmentation patterns of the mass spectra with those reported in the literature⁴⁹.

Statistical analyses

A dose-response analysis was done using a four-parameter log-logistic model (Eq. 2) (Alizadeh et al., 2020). The NLIN procedure of SAS software (Version 9.1) was used to plot the dry biomass of weed (y) against the ratios of species' dry aerial parts (flowers, leaves, and stems) residues (x).

$$y = a + \frac{(\max - \min)}{(1 + \exp(b * (\ln(x) - \ln(ED50))))} \text{Eq. 2}$$

where b is the slope of the curve at the $ED50$ point, $\min$ is the lower limit of the response curve at an infinitely large ratio of yarrow residues (weed biomass loss is almost zero when the ratio of yarrow residues application is maximum), $ED50$ is the amount of residues application that causes a 50% decrease in the dry weight of the weed, and $\max$ is the upper limit of the response curve (the maximum weed biomass when the amount of residues application is zero).

The effective doses necessary for a 10%, 50%, and 90% reduction in weed dry matter (*ED*10, *ED*50, and *ED*90) were computed after fitting the dose-response model. The following formulae (Eqs. 3 and 4) were substituted for *ED*50 in Eq. 1 to determine *ED*10 and *ED*90:

$$\exp [(\ln (ED10) - (1/b) \times \ln(1/9))] \text{ Eq. 3}$$

$$\exp [\ln (ED90) - (1/b) \times \ln(9)] \text{ Eq. 4}$$

The coefficient of determination (R^2) and root mean square error (RMSE) were employed to assess model efficacy (Eqs. 5 and 6).

$$R^2 = 1 - \frac{\sum_i^n [M_i - P_i]^2}{\sum_i^n [M_i - A_i]^2} \text{ Eq. 5}$$

$$RMSE = \sqrt{\left[\frac{\sum [P_i - M_i]^2}{n} \right]} \text{ Eq. 6}$$

P_i , M_i , and A_i are the values of the predicted, measured, and average dry weights of the weed, respectively, and n is the number of measuring points.

The partial least squares (PLS) regression was done by using the Microsoft Excel XLSTAT program (Version 2016). For PLS regression, the data included three dependent (response) variables, *ED*10, *ED*50, and *ED*90, and 81 independent (explanatory) variables, including the most important essential oil components identified in the five strongest allelopathic species. The study was carried out in stages, such as generating the correlation matrix among variables, assessing the model quality based on the number of components, and estimating model parameters to arrive at prediction equations for *ED*10, *ED*50, and *ED*90. Jackknife cross validation was carried out.

Statements on plant material

The plant material in this manuscript is legal and follows all relevant institutional, national, and international rules and laws. It can be obtained from various related centers around the world. The plants used are wild and were collected from natural habitats (pastures, mountains, and farmland margins). Dr. Mozaffarian then figured out what species they were by comparing them to vouchers from the Iran Research Institute of Forests and Rangelands in Tehran, Iran, and to the Iranian flora.

Statements on Data availability

The datasets used and/or analysed during the current study available from the corresponding author on reasonable request.

Declarations

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Author contributions statement

Gholamreza Niazipoor conceived and conducted the experiment, wrote the original draft; Majid AghaAlikhani was responsible for conceptualization, methodology and project management; Ali Mokhtassi-Bidgoli analyzed the results and revised the final draft; Sara Vitalini evaluate the original draft and recommended useful revisions. All authors reviewed the manuscript.

Competing interests

The authors declare no competing interests.

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Figures

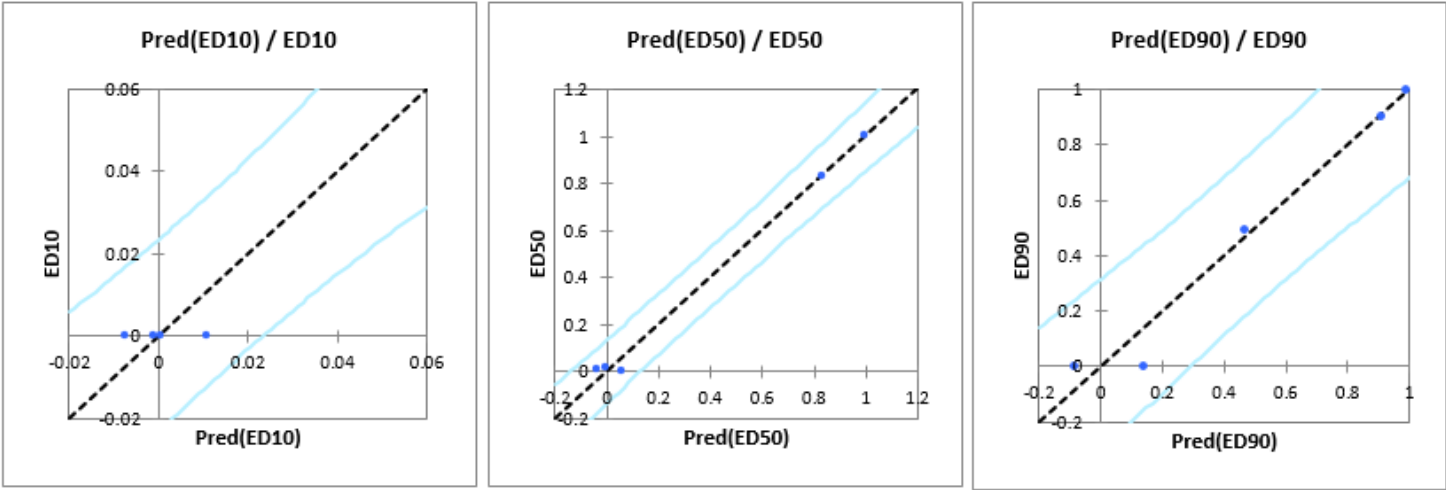


Figure 1

Measured versus predicted values (%) from the fitted PLS model at three *EDs*. The blue dots represent the measurement points, and the dotted line indicates predicted values at the *ED10*, *ED50*, and *ED90* of residual on redroot pigweed seedling growth.

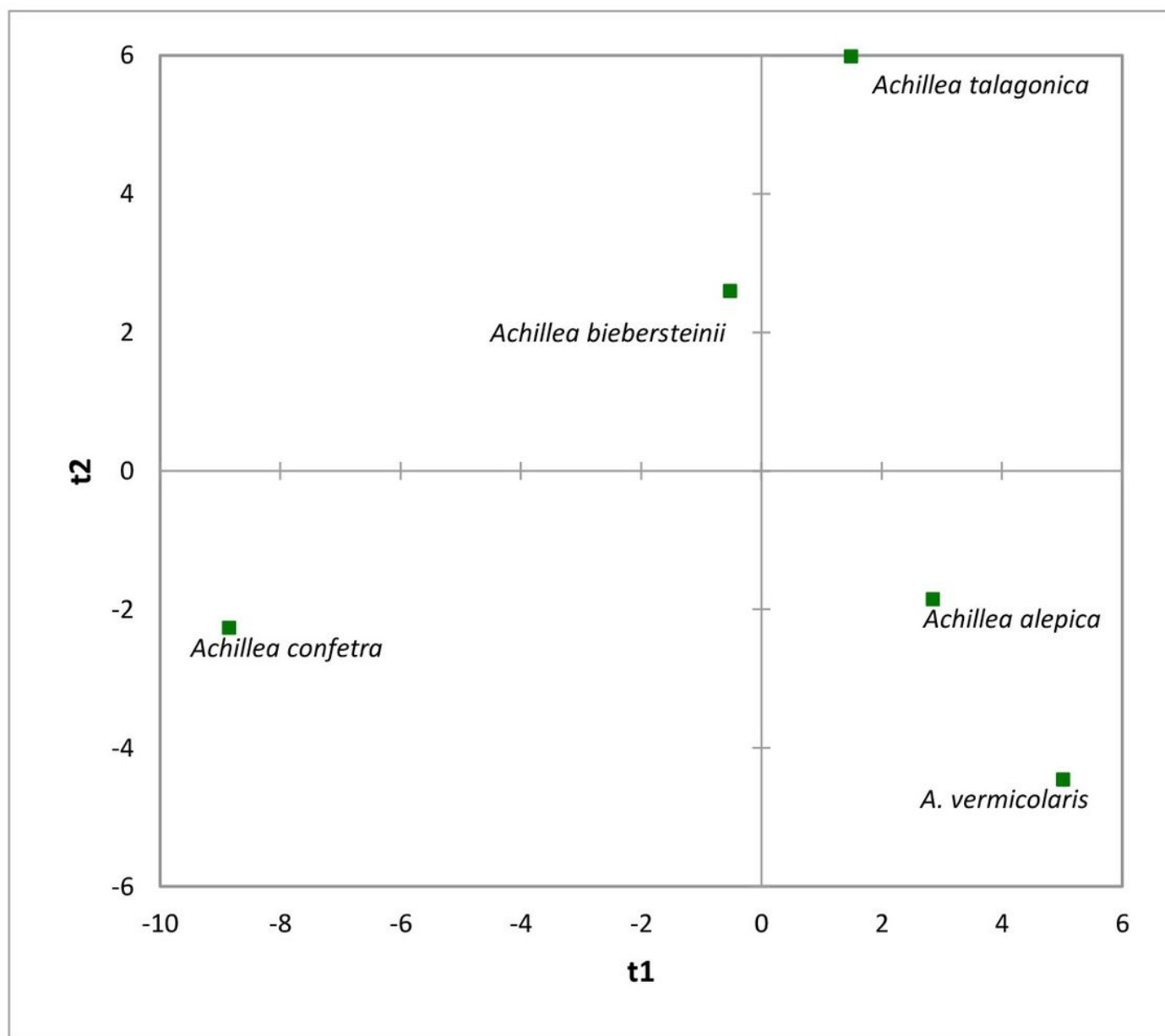


Figure 2

The similarity of the species in terms of the amount and type of essential oil compounds based on two PLS components (t_1 and t_2).

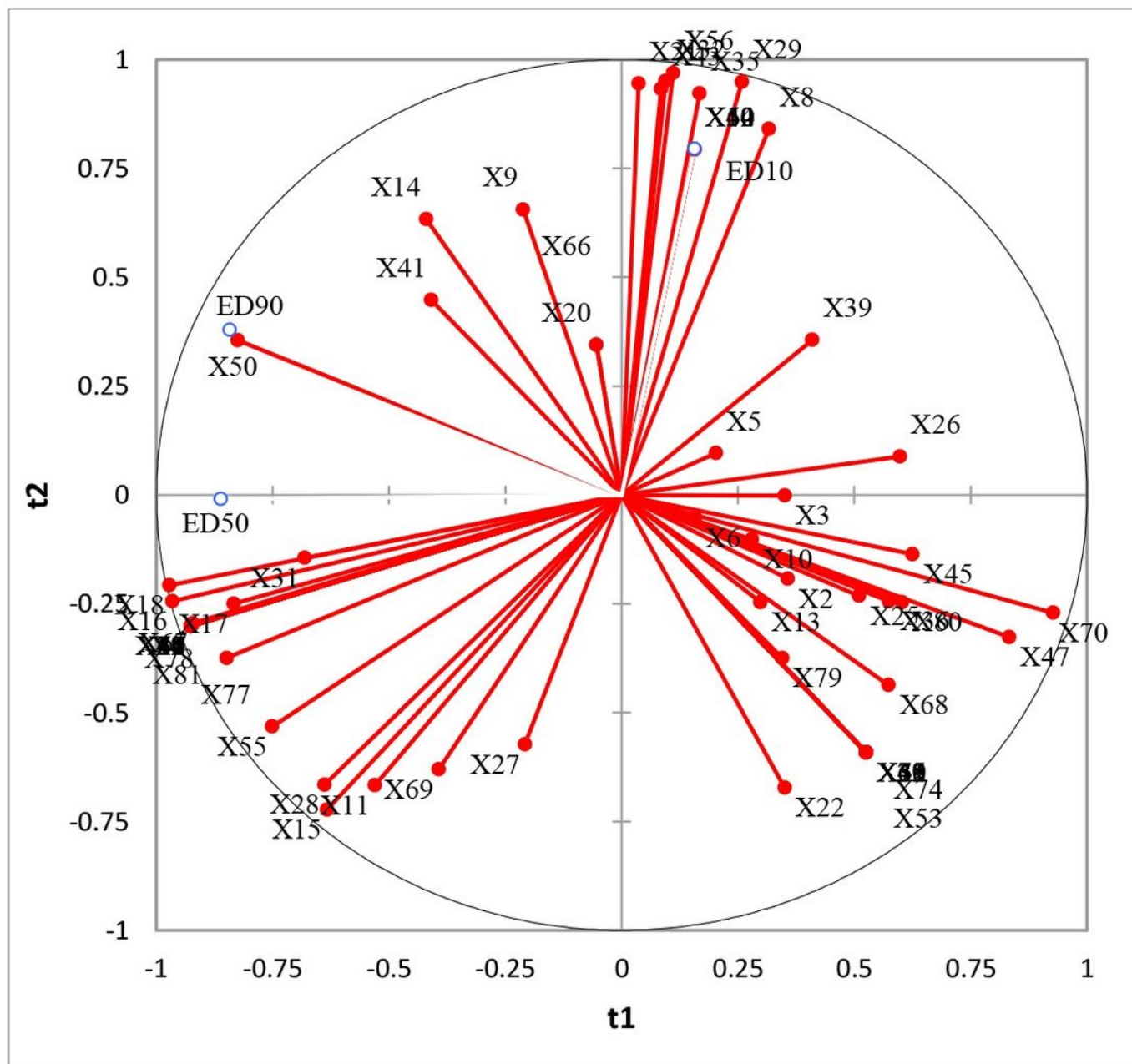


Figure 3

The relationships between allelochemicals at three effective doses (ED) in term of the first two PLS components. X1: Santolina triene, X2: α -Pinene, X3: campene, X4: sabinene, X5: β -Pinene; X6: 2,3-Dehydro-1,8-cineole, X7: Yomogi alcohol, X8: α -Phellandrene, X9: α -Terpinen, X10: p-Cymene, X11: β -Cymene, X12: o-Cymene, X13: Limonene, X14: 1,8-Cineole, X15: τ -Terpinen, X16: Sabinene hydrate, X17: Terpeneol, X18: cis- β - α -Thujone, X19: β -Thujone, X20: cis-Menth-2-en-1-ol, X21: p-Menth-2-en-1-ol, X22: Chrysanthenone, X23: Pinocarvone, X24: cis-Sabinol, X25: Camphor, X26: Pinocarvone, X27: Borneol, X28: Terpinen-4-ol, X29: Cryptone, X30: p-Cymen-8-ol, X31: α -Terpieol, X32: cis-Piperitol, X33: Fir Balsam Canada 20% RT12.582 SC937 RI1204 PR83 FG99, X34: Myrtenol, , X35: trans-Piperitol, X36: Carveol<trans->, X37: Ascaridole , X38: Chrysanthenyl acetate, X39: trans Piperitone, X40: Phellandral,

X41: Bornyl acetate, X42: Sabinyl acetate<trans->, X43: p-Cymen-7-ol, X44: Terpinene 4-acetate, X45: Thymol , X46: Tea-tree-EB-10pcent, X47: Carvacrol, X48: Carvyl, acetate<trans>, X49: α -Copaene , X50: Decanoic acid, X51: β -Elemene, X52: 3,5-Heptadienal, 2-ethylidene-6-methyl-,X53: Yarrow-blue-EB-10pcent RT17.709 SC1438 RI1398 PR78 FG90, X54: Jasmone, X55: Methyleugenol, X56: Caryophyllene, X57: β -Farnesene, X58: 2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7, X59: τ -cadinene, X60: β -Cubebene, X61: Germacrene D, X62: Selinene<beta>, X63: β -Ionone, X64: Bicyclogermacrene, X65: δ -Cadinene, X66: α -Terpinyl propionate, X67: Nerolidol, X68: Aromadendrene oxide-(2), X69: (-)-Spathulenol, X70: Caryophyllene oxide, X71: Aristolene epoxide, X72: Fokienol, X73: Aristolene epoxide, X74: 4-(4-Methylphenyl) pyridine , X75: unknown, X76: γ -Eudesmol, X77: β -Eudesmol, X78: Artemisia 7 04-06-12 20% RT23.558 SC2009 RI1625 PR86 FG98, X79: Palmitic acid, X80: Linolenic acid, X81: Linolenic acid and X82: methyl ester.