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Chemodiversity studies on *Cleome* L. genera by chemical characterization of *Cleome pallida* Kotschy and *C. fimbriata* Vicary essential oils with subsequent hierarchical cluster (HCA) and principal component analysis (PCA)

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Abstract: *Cleome* genus, belonging to the Cleomaceae family, distributed in several countries and many of which are used extensively. In fact, many of these specimens are consumed in the form of infusions or salads. In this study, the qualitative chemical composition of the essential oils obtained by hydrodistillation from *Cleome* ssp. was studied. Two species, two different accessions (**CP1**, and **CP2**) of *C. pallida* Kotschy, and one of *C. fimbriata* Vicary (**CF**), were collected in Oman and chemically investigated for the first time. The three essential oils were analyzed by gas chromatography and mass spectrometry (GC-MS). In total, 169 compounds were identified. Sesquiterpenoids were the major chemical group of **CP1** and **CP2** samples (56.4–58.8%); **CF**, instead, consisted essentially of nitrogen derivatives (30.2%), with 1-isothiocyanato-3-methylbutane (20.7%) as the most abundant class'. Furthermore, a new review of the chemical compositions' literature, never studied, was carried out on all other *Cleome* species. Statistical studies such as Hierarchical cluster (HCA) and principal component analysis (PCA) were used to establish chemo-similarities and to highpoint possible correlations between the chemical compositions of **CP1**, **CP2**, and **CF,** and the reported *Cleome* ssp. essential oils.

Keywords: Caryophyllene oxide, ecological traits, food properties, 1-isothiocyanato-3-methylbutane, volatile analyses

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1 Introduction

The genus *Cleome* L., the largest of Cleomaceae family, includes more than two-hundred species, growing in different regions of the Earth. *Cleome* species are annual or perennial bushy herbs or trees, and they are extensively distributed in tropical and sub-tropical regions (POWO, 2026).

Species of genus *Cleome* have a long history interest for human nutrition and health. The most utilized species is *C. gynandra* L., distributed in all Africa, India, Sri Lanka, Afghanistan, and Indochina. Leaf preparations are used to treat pain, epileptic fits, and ear infections and its decoction is utilized to treat constipation, conjunctivitis, worm infections, inflammation, etc. (Chand et al., 2022).

C. amblyocarpa Barratte & Murb. is an important medicinal herb with potential therapeutic applications in folk medicine. In the United Arab Emirates herbal medicine, infusions of leaves are used to treat abdominal and rheumatic pain (Sakkir et al., 2012) and against bacterial infections (Rahman et al., 2004). In Tunisia, this herb is widely used to ease pain and for the treatment of diabetes and colic (Edziri et al., 2013). It is mixed with other herbs to treat headaches, nausea, and vomiting (Tlig et al., 2012). *Cleome arabica* L., a closely related species, has been used in North African folk medicine for the treatment of various diseases such as stomachic therapy, rheumatic fever, scabies, and inflammation and it is also reported to have hallucinogenic properties (Bouriche & Arnhold, 2010). Fruits and leaves of *C. arabica* L. mixed with olive oil are used to make anti-inflammatory ointments in the Sahara region (Pullaiah, 2006). The same species in the Arabian Peninsula, where it is known as "Zafrah-Amal, Zambel, Shajarat-Aluahsh"; is used as carminative, appetizer and of tonic (Rahman et al., 2004).

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The whole plant and the vegetative parts (leaves, seeds, and roots) of *Cleome viscosa* Linn., commonly known as "wild or dog mustard," are widely used in Indian medicine with beneficial effects as an anthelmintic, antiseptic, carminative, antiscorbutic, sudorific, febrifuge, and cardiac stimulant (Mali, 2010; Gupta & Rao, 2012). *Cleome brachycarpa* Vahl ex DC. is utilized for rheumatism, scabies and inflammation, as well as an analgesic agent against pain in lower abdomen in the indigenous systems of medicine in West Africa (Viqar & Khisal, 1987). It is also used in Ayurvedic medicine, and its properties have been reviewed (Naeem et al., 2019). *Cleome rutidosperma* DC. is an annual African herb which has naturalized in Tropical America and Asia. Traditionally, in Nigeria, the plant is used for the treatment of paralysis, epilepsy, convulsions, spasm, earache and fungal infections (Morah & Apebende, 2018). In West and East Africa, the young shoots and leaves of this plant are boiled and consumed as a green vegetable. Furthermore, the roots are popularly used for their analgesic, anti-inflammatory, and wound healing properties (McNeil et al., 2018). Its traditional uses have been recently reviewed (Ghosh et al., 2019). *Cleome droserifolia* (Forssk.) Delile, a plant growing in Egyptian and Jordan deserts, it is used in traditional medicine as a hypoglycaemic agent and for the treatment of diabetes mellitus type 2 (Abd El-Gawad et al., 2018; Abdel-Kawy et al., 2000). *C. khorassanica* Bunge & Bien. ex Boiss. was used in Iran and Afghanistan an antispasmodic, diuretic, laxative and to treat respiratory problems such as asthma and bronchitis and eczema and psoriasis (Joukar et al., 2024a). Similar activities have been reported for *C. spinosa* Jacq. in Brazil (dos Santos Magalhães et al., 2023).

In the context of effective agriculture and nutritional security, among underutilized indigenous crops these, also species of the genus *Cleome* have emerged as promising candidates due to their dual functionality as both nutrient-rich leafy vegetables and effective cover crops. Widely cultivated across Africa and Asia, *Cleome* species have been historically utilized as food for human consumption whereas many others have been totally neglected (Mashamaite et al., 2022).

Cleome gynandra is the species most used as food. Its leaves and shoots are eaten boiled or in stews and in Africa, or fermented in Thailand and Malaysia (Pieroni, 2005; Waithaka & Chweya, 1991). In Eastern and Southern Africa, the young shoots of *Cleome hirta* (Klotzsch) Oliv. and *Cleome monophylla* L. are cooked and used like spinach (Burkill, 1985). The use of *C. viscosa* in Nepal has been largely reported. Its leaves and young shoots are cooked and eaten as vegetable whereas the seeds can be pickled or used as a mustard substitute in curries (Manandhar, 2002).

Despite their potential, *Cleome* species remain underexploited in mainstream agricultural systems and the assessment of their role in sustainable food systems, and their relevance in addressing food security and ecological challenges in resource-constrained environments remains to be investigated (Giacalone et al., 2021).

Due to their interesting biological properties many papers were published on the isolation and characterization of non-volatile metabolites occurring from different species of *Cleome* genus. The principal groups of compounds were: terpenoids, flavonol glycosides, coumarino-lignoids, dipyridodiazepinones and isothiocyanate derivatives. Isothiocyanates, a class of compounds predominantly found in cruciferous plants such as broccoli, cauliflower, kale, cabbage, watercress, and other vegetables (Olayanju et al., 2024). Isothiocyanates are phytochemicals with several biological activites. Bioactivity includes the stimulation of cellular antioxidant systems, induction of apoptosis and interference with cytokine production and activity. Furthermore, epidemiological evidence and experimental studies indicate that naturally occurring isothiocyanates and synthetic derivatives have anti-cancer and anti-inflammatory properties (Brown & Hampton, 2011). Several comprehensive reviews on the occurrence of non-volatile compounds as well as on the biological properties of *Cleome* species were published (Chand et al., 2022; Abdullah et al., 2016; Singh et al., 2018).

With regards to the composition of the essential oils (EOs) of species of this genus, several papers were published and a complete review, not present in literature, has been carried out in this work.

Cleome pallida Kotschy (Figure S1), whose native habitat is Egypt to Somalia and NW India, is a subshrub and grows primarily in the desert or dry shrub-land biome (POWO, 2026). It has several synonymous and for a long time it has been attributed to the monotypic genus *Dipterygium* with the name *Dipterygium glaucum* Decne. Later this species was moved to genus *Cleome* (Hedge & Lamond, 1970). It is a xeromorphic species resistant environmental stress conditions. In fact, it lives in severe aridity and rarity of water. *Cleome pallida* Kotschy is a plant up to 0.6 m tall, from a woody base; stems are slender, sparsely, and branched. Leaf-blades are oblong or elliptic, with sessile or subsessile glands on both surfaces. Sepals up to 1 mm long, petals are pale-yellow fading whitish, often tinged violet, 3–4 mm long; Fruit are winged, rugose or crested fruit-body (Wood, 1997).

C. pallida, although its use as food was not reported, is an important medicinal plant utilized to cure skin diseases, respiratory diseases, wounds and chronic fever (Malik et al., 2015). It is largely utilized by the Bedouins in Saudi Arabia for the treatment of miss-breathing troubles as trachea dilating agent (Abdel-Mogib et al., 2000). A decoction and infusion of the plant is used in the traditional medicine of Pakistan to treat jaundice, ringworm infestation, psoriasis, and as blood purifier antiasthma drug (Rahman et al., 2004; Ahmad et al., 2014). The occurrence, in *C. pallida*, of several non-volatile metabolites such as cyanides, coumarins, alkaloids, and flavonoids, and several biological activities like antioxidant, anti-inflammatory, antidiabetic, anti-Alzheimer, insecticidal, anthelmintic, antileishmanial, antibacterial and antifungal were reported (Moussa et al., 2012; Hameed et al., 2011; Shaheen et al., 2017; Choudhary et al., 2019; Shahid et al., 2023). Nothing has been published on the chemical composition of its essential oil.

Cleome fimbriata Vicary [Syn: *Cleome noeana* Boiss., *Cleome noeana* var. *hispida* Regel & Schmalh., *Cleome noeana* var. *persepolitana* Bornm., *Cleome griffithiana* Rech.f., *Cleome quinquenervia* var. *noeana* (Boiss.) Parsa,

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Rorida fimbriata (Vicary) Khorasani & Naqinezhad] (Figure S2) grows primarily in the tropical habitat. The native range of this species is Arabian Peninsula Iraq to S. Asia and NW. India (POWO, 2026). *Cleome fimbriata* Vicary is an annual or perennating herb 30–60 cm tall; the leaves are simple, suborbicular to broadly ovate; fruits are conspicuously linear, 20–30 mm long; seeds are many, about 1 mm in diam., glabrous, minutely granulate, brownish (Wood, 1997).

To the best of our knowledge this is the first study on *Cleome pallida* Kotschy and *C. fimbriata* Vicary volatiles. Herein, not only the volatile composition but also the statistical PCA and HCA were performed for the first time to obtain possible chemotaxonomic correlations between the various *Cleome* species.

2 Materials and Methods

2.1 Plant Materials

Aerial parts (flower, leaves, and stems) of *Cleome pallida* (Figure S1) were collected in two different locations: at Al Raka, in a sandy desert, Oman (22°24′56″ N 58°47′09″ E 291 m s.l.) on the 27th February 2025, and near Haima, in a rocky-desert environment, Oman (19°56′36″ N 56°17′35″ E 124 m s.l.) on the 1st March 2025. Samples, identified by Prof. Vincenzo Ilardi, have been stored in the Herbarium Mediterraneum Panormitanum (PAL), (Voucher No. 109787 and No. 109786, respectively), of the Botanical Garden of the University of Palermo, Italy.

Aerial parts (flower, leaves, and stems) of *Cleome fimbriata* (Figure S2) were collected near Dauka, Oman (18°26′38″ N 54°03′45″ E 256 m s.l.) on the 1st March 2025. Samples, identified by Prof. Vincenzo Ilardi, have been stored in the Herbarium Mediterraneum Panormitanum (PAL), (Voucher No 109788), of the Botanical Garden of the University of Palermo, Italy.

2.2 Extraction of Volatile Components

Fresh aerial parts (flower, leaves, and stems) of the two accessions of *C. pallida* (223 g and 105 g, respectively), and of *Cleome fimbriata* (300 g), were ground in a Waring blender and then subjected to hydrodistillation for 3 h, according to the procedure described in European Pharmacopoeia 10.3 (2020). All essential oils were dried over anhydrous sodium sulphate and stored in a sealed vial under N_2, at −20°C, ready for GC-MS analyses.

2.3 GC-MS Analysis

Analyses of essential oils were performed, assingle injection, as reported by Lauricella et al. (2022). GC-MS analysis was performed using a Shimadzu QP 2010 GC-MS analysis was performed using a Shimadzu QP 2010 plus equipped with an AOC-20i autoinjector (Shimadzu, Kyoto, Japan) gas chromatograph equipped with a capillary column (DB-5 MS) of 30 m × 0.25 mm i.d., film thickness 0.25 µM, and a data processor. The oven program was as follows: temperature was held at 40°C for 5 min, then increased at a rate of 2°C/min up to 260°C, then isothermal for 20 min. Helium was used as carrier gas (1 mL min^{-1}). The injector and detector temperatures were set at 250 and 290°C, respectively. One µL of essential oil solution (3% essential oil/hexane *v/v*) was injected in split mode 1:50; MS range 40–600. The settings were as follows: ionization voltage, 70 eV; electron multiplier energy, 2000 V; transfer line temperature, 295°C; solvent delay, 3 min.

The relative percentages (%) listed in Table 1 were calculated using the area of peaks from chromatogram. The identification of peaks was carried out by comparison with their mass spectra and relative retention indices with WILEY275, NIST 17, ADAMS, and FFNSC2 commercial libraries and by using Linear Retention Indices (LRI).

2.4 Statistical Analysis

To evaluate chemo-similarities, distinctive chemical classes such as those of monoterpene hydrocarbons (**MH**), oxygenated monoterpenes (**OM**), sesquiterpene hydrocarbons (**SH**), oxygenated sesquiterpenes (**OS**), diterpenes (**D**), organic acids and esters (**AE**), nitrogen derivatives (**ND**), and other compounds (**O**). Chemical classes were considered as original variables and subjected, after normalization, to cluster analysis (CA) and to Principal Component Analysis (PCA).

The statistical analyses were performed using PRIMER 6 (Massey University East-bourne, Albany, New Zealand) (Clarke & Gorley, 2006) with two principal components (PC1 and PC2) variables and the number of clusters were determined by using the rescaled distances in the dendrogram, using two cut-off point (Euclidean distance = 1, and 2) that allows the attainment of consistent clusters. Principal component analysis (PCA) was performed using the correlation matrix method with sequential eigenvalues selected after normalization. The varimax rotation method was used to improve the correlation between chemical constituents and principal components, not scaling the data in the graphical representation. Correlation matrices were used to assess the effect of different constituents on chemotypes. The PCA and the Hierarchical Cluster Analysis (HCA) were used to comprehend the similarity among the essential oils in relation to the contents of their principal chemical classes. Since the HCA analysis is a function of variables and observations, the highest correspondence between PCA and HCA resulted when we applied a cut-off of 1 and 2.

3 Results and Discussion

3.1 Essential Oils Composition

Hydrodistillation of *C. pallida* aerial parts, collected at Al Raka, Oman, gave a pale-yellow oil (**CP1**, yield 0.02%). Overall, eighty-five compounds were identified, representing 96.1% of total components, listed in Table 1 according to their linear retention indices on a DB-5MS column and classified into eight classes based on their chemical structures. Sesquiterpene hydrocarbons (32.1%) were the principal class with *γ*-himachalene (5.9%) as the main constituent. Oxygenated sesquiterpenes, the second most abundant class (24.2%), showed a large quantity of guaiol (17.8%), the most

Table 1. Chemical composition (%) of *Cleome pallida* essential oils collected in Al Raka (**CP1**) and Haima (**CP2**), and *Cleome fimbriata* in Dauka (**CF**), Oman

No.	Compounds[a]	LRI[b]	LRI[c]	CP1	CP2	CF	Identification
1	**α-Pinene**	930	931	1.8	0.9	**5.8**	MS, LRI, I
2	Camphene	943	947	0.2	0.5	–	MS, LRI, I
3	**β-Pinene**	**977**	**975**	**6.1**	–	**5.4**	MS, LRI, I
4	2,3-Dehydro-1,8-cineole	987	986	–	–	0.4	MS, LRI
5	β-Myrcene	990	992	–	1.6	–	MS, LRI, I
6	α-Phellandrene	1001	1003	–	2.2	0.2	MS, LRI
7	4-Carene	1012	1014	–	0.8	–	MS, LRI
8	α-Terpinene	1013	1016	–	–	0.3	MS, LRI, I
9	*p*-Cymene	1020	1022	0.1	1.6	0.6	MS, LRI, I
10	Limonene	1025	1028	0.5	2.8	0.9	MS, LRI, I
11	*Trans*-Ocimene	1037	1038	–	0.1	–	MS, LRI, I
12	*Cis*-Ocimene	1047	1043	–	0.1	–	MS, LRI, I
13	γ-Terpinene	1055	1055	0.1	0.2	–	MS, LRI, I
14	Terpinolen	1085	1088	0.1	0.1	–	MS, LRI, I
15	Dehydro-*p*-cymene	1087	1090	–	–	0.4	MS, LRI
16	1,1-Dimethyl-3-methylene-2-vinylcyclohexane	1116	1118	–	–	0.4	MS, LRI
	Monoterpene Hydrocarbons			**8.9**	**10.9**	**14.4**	
17	2-Methyl-6-methylen-octa-1,7-dien-3-one	1096	1103	–	–	0.1	MS, LRI
18	β-Linalool	1099	1098	0.5	0.4	–	MS, LRI, I
19	α-Campholenal	1121	1125	–	–	0.3	MS, LRI
20	(*E*)-3(10)-Caren-4-ol	1129	1134	–	–	0.2	MS, LRI
21	Isopinocarveol	1132	1132	0.1	–	–	MS, LRI
22	*Trans*-Pinocarveol	1134	1135	–	–	0.8	MS, LRI
23	*Cis*-Verbenol	1140	1141	0.1	–	0.3	MS, LRI, I
24	*Trans*-Verbenol	1141	1145	–	–	0.6	MS, LRI, I
25	Epoxylinalol	1144	1136	–	–	0.2	MS, LRI
26	α-Pinocarvone	1156	1164	–	–	0.6	MS, LRI
27	Borneol	1160	1162	0.1	–	–	MS, LRI, I
28	α-Phellandren-8-ol	1163	1167	–	–	0.3	MS, LRI
29	β-Pinanone	1167	1169	–	–	0.2	MS, LRI
30	4-Terpineol	1172	1177	0.2	0.1	1.5	MS, LRI, I
31	*p*-Cymen-8-ol	1182	1183	–	–	0.7	MS, LRI, I
32	α-Terpineol	1187	1189	0.5	0.1	0.4	MS, LRI, I
33	Myrtenol	1189	1192	–	–	0.3	MS, LRI
34	Safranal	1193	1201	0.1	–	–	MS, LRI
35	Myrtenal	1194	1198	–	–	1.2	MS, LRI, I
36	Verbenone	1202	1207	–	–	0.1	MS, LRI
37	β-Cyclocitral	1214	1224	0.1	*t*	–	MS, LRI
38	*Cis*-Carveol	1215	1215	–	-	0.3	MS, LRI
39	Nerol	1226	1229	0.1	*t*	–	MS, LRI, I
40	Thymol methyl ether	1231	1325	–	*t*	–	MS, LRI, I
41	Neral	1237	1239	–	0.1	–	MS, LRI, I
42	*p*-Menth-8(10)-ene-2,9-diol	1247	1251	–	–	0.1	MS, LRI
43	Geraniol	1254	1255	0.2	*t*	–	MS, LRI, I
44	Verbenyl acetate	1258	1262	–	0.1	–	MS, LRI
45	5-Methoxyindole	1265	1269	–	–	1.0	MS, LRI
46	(*E*)-Geranial	1266	1268	–	0.1	–	MS, LRI
47	Isobornyl acetate	1282	1288	–	0.1	–	MS, LRI
48	(*Z*)-Geranial	1285	1289	–	0.1	–	MS, LRI
49	Dihydroedulan I	1287	1293	–	0.1	–	MS, LRI
50	*p*-Cumin-7-ol	1292	1295	–	–	0.2	MS, LRI

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Table 1. (Continued)

No.	Compounds[a]	LRI[b]	LRI[c]	CP1	CP2	CF	Identification
51	*Trans*-Pinocarveol	1296	1298	–	–	0.1	MS, LRI
52	4-Vinylguaiacol	1306	1311	–	*t*	–	MS, LRI
53	Myrtenyl acetate	1322	1322	–	–	0.3	MS, LRI
54	Eugenol	1353	1356	0.3	*t*	–	MS, LRI, I
55	Geranyl acetate	1385	1386	0.1	0.6	–	MS, LRI
56	Methyl eugenol	1401	1401	–		0.3	MS, LRI, I
	Oxygenated Monoterpens			**2.4**	**1.8**	**10.1**	
57	*α*-Cubebene	1347	1351	0.1	0.5	0.2	MS, LRI
58	Ylangene	1363	1361	0.4	0.1	–	MS, LRI
59	*β*-Cubebene	1375	1381	1.5	0.8	0.3	MS, LRI
60	*α*-Bourbonene	1381	1383	0.2	0.3	–	MS, LRI
61	*β*-Cubebene	1386	1385	–	0.3	–	MS, LRI
62	*β*-Elemene	1391	1394	0.1	*t*	–	MS, LRI
63	*α*-Gurjunene	1396	1402	1.1	0.3	–	MS, LRI
64	*β*-Gurjunene	1400	1402	–	0.1	–	MS, LRI
65	Caryophyllene	1407	1408	3.4	0.2	–	MS, LRI, I
66	*β*-Maaliene	1414	1415	–	1.0	–	MS, LRI
67	Humulen-(v1)	1420	1418	3.3	–	–	MS, LRI
68	*α*-Muurolene	1426	1435	0.2	0.2	–	MS, LRI
69	*γ*-Elemene	1430	1431	–	0.2	–	MS, LRI
70	*α*-Bergamotene	1436	1438	1.1	0.5	–	MS, LRI
71	*β*-Sesquiphellandrene	1443	1443	0.5	0.2	–	MS, LRI
72	6-epi-*β*-Cubebene	1445	1445	–	0.4	–	MS, LRI
73	1,1,4,8-Tetramethyl-4,7,10-cycloundecatriene	1447	1447	–	0.3	–	MS, LRI
74	*β*-Farnesene	1452	1455	1.9	0.1	–	MS, LRI
75	Humulene	1457	1459	1.7	1.6	–	MS, LRI, I
76	Aristolene	1466	1460	0.6	–	–	MS, LRI
77	*γ*-Gurjunene	1469	1469	0.5	0.4	0.2	MS, LRI
78	*β*-Cubebene	1472	1474	–	–	0.7	MS, LRI
79	Valencene	1474	1472	1.1	1.5	0.4	MS, LRI
80	*α*-Bourbonene	1480	1484	–	–	1.2	MS, LRI
81	*β*-Eudesmene	1482	1484	–	1.4	–	MS, LRI
82	***γ*-Himachalene**	1488	1494	**5.9**	0.7	–	MS, LRI
83	*α*-Selinene	1495	1493	1.1	1.0	1.3	MS, LRI
84	Zingiberene	1496	1497	–	1.3	–	MS, LRI
85	*β*-Muurolene	1503	1499	3.3	1.7	0.8	MS, LRI
86	*β*-Bisabolene	1509	1510	1.4	1.4	1.2	MS, LRI, I
87	Selina-3,7(11)-diene	1518	1522	0.3	–	–	MS, LRI
88	***δ*-Cadinene**	1524	1529	1.7	**6.2**	1.5	MS, LRI
89	(*E*)-Cadina-1,4-diene	1530	1533	–	0.5	0.3	MS, LRI
90	*γ*-Cadinene	1534	1536	–	0.6	0.2	MS, LRI
91	*α*-Calacorene	1539	1538	0.4	0.2	0.7	MS, LRI
92	Cadala-1(10),3,8-triene	1558	1562	0.3	0.3	0.5	MS, LRI
93	Cadalene	1668	1668	–	–	0.3	MS, LRI
	Sesquiterpene Hydrocarbons			**32.1**	**24.3**	**9.8**	
94	Elemol	1548	1549	1.0	–	–	MS, LRI
95	Longifolebaldehyde	1550	1563	–	–	0.4	MS, LRI
96	*Trans*-Nerolidol	1565	1565	0.7	–	0.1	MS, LRI, I
97	**Caryophyllene oxide**	1580	1578	1.6	**19.8**	1.6	MS, LRI, I
98	Globulol	1596	1597	–	0.4	–	MS, LRI
99	Diepicedrene-1-oxide	1604	1596	0.4	–	1.0	MS, LRI

Table 1. (Continued)

No.	Compounds[a]	LRI[b]	LRI[c]	CP1	CP2	CF	Identification
100	Carotol	1610	1614	–	0.3	0.2	MS, LRI
101	*α*-Cubenol	1613	1611	–	0.7	1.6	MS, LRI
101	*α*-Cubenol	1613	1611	–	0.7	1.6	MS, LRI
102	*β*-Cubenol	1626	1628	–	1.1	–	MS, LRI
103	*τ*-Cadinol	1643	1640	–	4.1	3.1	MS, LRI
104	**Guaiol**	1641	1646	**17.8**	0.6	1.4	MS, LRI
105	Agarospirol	1650	1646	0.4	0.3	–	MS, LRI
106	*β*-Eudesmol	1657	1649	1.3	4.8	3.0	MS, LRI
107	*Epi*-*α*-Elemol	1679	1668	0.4	0.4	–	MS, LRI
108	Lanceol	1744	1753	–	0.2	–	MS, LRI
109	Aristolone	1797	1787	0.6	–	–	MS, LRI
	Oxygenated Sesquiterpenes			**24.2**	**32.7**	**12.4**	
110	Rimuene	1911	1914	–	–	1.1	MS, LRI
111	Beyerene	1917	1921	–	–	0.9	MS, LRI
112	α-Springene	1955	1962	–	–	1.1	MS, LRI
113	(*E*,*E*)-Geranyllinalool	2014	2020	1.1	–	–	MS, LRI
114	(*Z*,*Z*)-Geranyllinalool	2034	2036	1.0	–	–	MS, LRI
115	Phytol	2112	2110	1.1	0.5	–	MS, LRI, I
116	Verticiol	2172	2176	–		4.1	MS, LRI
117	3-Ethyl-3-hydroxyandrostan-17-one	2252	2256	–	–	2.8	MS, LRI
	Diterpenes			**3.2**	**0.5**	**10.0**	
118	Methyl (3*Z*)-3,7-dimethyl-3,6-octadienoate	1274	1277	–	*t*	–	MS, LRI
119	Decanoic acid	1395	1393	–	–	1.8	MS, LRI, I
120	Ethyl cinnamate	1459	1460	–	–	0.4	MS, LRI
121	Dodecanoic acid	1576	1581	–	–	1.0	MS, LRI, I
122	Tetradecanoic acid	1768	1767	–	0.6	1.5	MS, LRI, I
123	Pentadecanoic acid	1863	1865	–	0.3	0.6	MS, LRI, I
124	Methyl hexadecanoate	1926	1927	1.5	0.3	0.2	MS, LRI
125	**Hexadecanoic acid**	1987	1987	**6.7**	**10.0**	3.0	MS, LRI, I
126	Ethyl palmitate	1998	1999	1.5	0.5	0.4	MS, LRI, I
127	Methyl linolate	2092	2092	0.6	0.3	–	MS, LRI, I
128	Methyl linolenate	2099	2098	1.0	0.6	–	MS, LRI, I
129	Linoleic acid	2134	2134	–	3.4	–	MS, LRI, I
130	(*Z*)-6-Octadecenoic acid	2144	2147	–	0.6	–	MS, LRI
131	Ethyl linolate	2159	2159	2.0	0.5	–	MS, LRI, I
132	Ethyl linolenate	2166	2169	2.5	0.9	–	MS, LRI, I
133	Ethyl stearate	2197	2194	0.4	–		MS, LRI, I
	Esters and Organic Acids			**16.2**	**18.0**	**8.9**	
134	Isocaponitrile	850	848	–	–	5.5	MS, LRI
135	Isobutyl isothiocyanate	947	946	–	–	1.5	MS, LRI
136	**1-Isothiocyanato-3-methylbutane**	**1069**	**1062**	–	–	**20.7**	MS, LRI
137	Isothiocyanatehexane	1161	1169	–	–	0.7	MS, LRI
138	Indole	1285	1292	–	–	0.7	MS, LRI
139	Benzyl Isothiocyanate	1355	1359	–	–	0.3	MS, LRI
	Nitrogen Derivatives			–	–	**29.4**	
140	2-Ethylfuran	776	778	0.1	–	–	MS, LRI
141	2,4-Dimethyl-3-pentanol	784	789	0.3	–	–	MS, LRI
142	Hexanal	819	814	0.5	–	–	MS, LRI, I
143	(*E*)-2-Hexanal	821	825	0.5	–	–	MS, LRI, I

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Table 1. (Continued)

No.	Compounds[a]	LRI[b]	LRI[c]	CP1	CP2	CF	Identification
144	3-Hexen-1-ol	843	844	1.0	–	–	MS, LRI, I
145	1-Hexanol	875	878	1.7	–	–	MS, LRI, I
146	1-Nonene	892	894	–	0.4	–	MS, LRI
147	1-Octen-3-ol	979	979	0.1	–	–	MS, LRI
148	3-Octanone	985	985	0.2	–	–	MS, LRI
149	2-Pentylfuran	991	996	0.4	–	–	MS, LRI
150	3-Octanol	996	998	0.4	–	–	MS, LRI
151	Benzeneacetaldehyde	1036	1039	0.2	0.1	–	MS, LRI, I
152	1-Octanol	1071	1073	0.1	0.1	0.1	MS, LRI, I
153	1-Undecene	1091	1090	–	*t*	–	MS, LRI
154	Undecane	1101	1100	–	0.1	–	MS, LRI, I
155	Nonanal	1102	1102	0.2	–	0.1	MS, LRI, I
156	Dodecane	1201	1200	–	0.2	–	MS, LRI, I
157	Decenal	1203	1208	–	0.1	0.1	MS, LRI, I
158	1-Decanol	1272	1276	0.1	–	–	MS, LRI
159	Tridecane	1301	1300	0.1	0.2	–	MS, LRI, I
160	(*E*,*E*)-2,4-decadienal	1311	1314	–	0.1	–	MS, LRI
161	4,11-Dimethyl-tetradecane	1464	1466	–	0.1	–	MS, LRI
162	Pentadecanal	1715	1715	0.5	–	–	MS, LRI, I
163	Hexahydrofarnesyl acetone	1845	1839	0.5	0.6	0.9	MS, LRI, I
164	(9*E*,12*E*,15*E*)-9,12,15-Octadecatrien-1-ol	2150	2154	1.6	–	–	MS, LRI
165	Tricosane	2301	2300	0.3	0.2	–	MS, LRI, I
166	Pentacosane	2501	2500	0.3	0.5	–	MS, LRI, I
167	Hexacosane	2602	2600	–	0.3	0.4	MS, LRI, I
	Others[e]			**9.1**	**3.0**	**1.6**	
	Total			**96.1**	**91.2**	**96.6**	

Note: [a]Components listed in order of elution on a DB-5MS apolar column; [b]LRIs based on literature (https://webbook.nist.gov/), [c]Experimental LRIs on a DB-5MS apolar column; [d]Identification was performed by comparison with mass (MS), linear retention indices (LRI), and injection of pure standards (I); [e]This class included alkanes, alcohols, aldehydes, ketones, and possibly aromatic compounds.

abundant metabolites of this oil. Among the monoterpene hydrocarbons (8.9%), only β-pinene occurred in significant amount (6.1%), whereas hexadecanoic acid (6.7%) was the main compound among the esters and organic acids class (16.2%). The oil was totally devoid of nitrogen derivatives and showed a quite low amount of diterpenoids (3.2%).

Hydrodistillation of the aerial parts of the other accesion of *C. pallida*, collected at Haima, Oman, gave a yellow oil (**CP2**, yield 0.02%). Overall, ninety-six compounds were identified, representing 91.2% of total components, listed in Table 1. Its profile was quite similar to **CP1** although, in this case, oxygenated sesquiterpenes (32.7%) represented the main class with caryophyllene oxide (19.8%), a metabolite poorly represented in **CP1** (1.6%), as most abundant component of the oil. Sesquiterpene hydrocarbons (24.3%) was the second most abundant class, with δ-cadinene (6.2%) as principal metabolites. Among the monoterpene hydrocarbons (10.9%), devoid of β-pinene, only limonene (2.8%) and α-phellandrene (2.2%) occurred in moderate amount. **CP2** showed, as **CP1**, to be totally devoid of nitrogen derivatives, and a very low amount of diterpenoids (0.5%). Similarly to **CP1**, hexadecanoic acid (10.0%) was, in **CP2**, the main compond among the esters and organic acids (18.0%).

Hydrodistillation of *C. fimbriata* aerial parts, collected at Dauka, Oman, gave a pale-yellow oil (**CF**, yield 0.02%). Overall, eighty-two compounds were identified, representing 96.6% of total components, listed in Table 1. The chemical profile of **CF** totally differs from **CP1** and **CP2**. In fact, nitrogen derivatives (29.4%), absent in **CP1** and **CP2**, was the main metabolite class, with 1-isothiocyanato-3-methylbutane (20.7%) and isocaponitrile (5.5%) as principal contituents. The good amount of diterpenoids (10.0%) is also noteworthy, being verticiol (4.1%) the principal component. Among all the other terpenoids [monoterpenes (24.5%) and sesquiterpenes (22.2%)], only β-pinene and α-pinene were present in significant amount (5.4% and 5.8%, respectively).

The chemical composition of **CP1**, characterized by the modest quantity of α-pinene, β-himalachene, guaiol, and hexadecanoic acid, does not find similarities with other essential oils obtained from other *Cleome* species (Table 2); **CP2**, however, due to the respectable presence of caryophyllene oxide, and the low percentage of hexahydrofarnesyl acetone, presented certain similarities with the essential oil

Table 2. Main aerial parts components and chemical classes of *Cleome* essential oils obtained by hydrodistillation and reported in literature

Acronym	Taxa	Origin[a]	Essential oils' main compounds	MH	OM	SH	OS	D	AE	ND	O	Reference
CA1	*C. amblyocarpa* Barratte & Murb.	Egypt fl, May	Caryophyllene oxide (36.0%), hexahydrofarnesyl acetone (7.9%), alloaromadendrene epoxide (6.2%)	0	8.7	15.1	60.7	0.2	0.2	0	12.3	Abd-El-Gawad et al. (2021)
CA2	*C. amblyocarpa* Barratte & Murb.	Saudi Arabia fl, April	2-methoxy-4-vinyl phenol (20.1%), *cis*-dihydro carvone (13.1%), *β*-cubebene (7.5%)	3.6	18.9	16.7	5.7	0	3.6	3.9	46.3	Al-Humaidia et al. (2019)
CA3	*C. amblyocarpa* Barratte & Murb.	UAE, CLWS nr	Isobornyl formate (43.9%), tetrahydro-linalool acetate (7.4%), *neo*-menthyl acetate (5.8%)	0	66.1	5.3	0	0	4.0	2.0	22.5	Shahin et al. (2018)
CA4	*C. amblyocarpa* Barratte & Murb.	UAE, CMWS nr	Isobornyl formate (38.6%), tetrahydrolinalool acetate (6.3%), verbenone (5.9%)	0	66.9	9.4	0	0	6.4	0	17.3	Shahin et al. (2018)
CA5	*C. amblyocarpa* Barratte & Murb.	UAE, CHWS nr	*β*-ocimenone (39.6%), *γ*-elemene (8.3%), methyl eugenol (7.41%)	0	71.1	10.7	0	0	2.6	0	8.5	Shahin et al. (2018)
CU	*C. austroarabica* D. F. Chamb. & Lamond	Oman nr November	Thunbergol (36.7%), *β*-eudesmol (14.0%), *α*-eudesmol (10.4%)	2.2	1.2	12.2	38.2	36.7	0	1.6	5.0	Rehman et al. (2021)
CB1	*C. brachycarpa* Vahl ex DC.	Pakistan, Kot Musa fl October	*γ*-eudesmol (37.5%), elemol (24.9), *α*-caryophyllene (13.7%)	2.3	9.9	16.8	66.9	0	0	0	0	Baloch et al. (2025)
CB2	*C. brachycarpa* Vahl ex DC.	Pakistan, Ramak fl October	*γ*-eudesmol (37.8%), elemol (25.4), *α*-caryophyllene (14.1%)	2.9	9.7	17.2	67.9	0	0	0	0	Baloch et al. (2025)
CB3	*C. brachycarpa* Vahl ex DC.	Pakistan, Bhakkar fl October	*γ*-eudesmol (37.0%), elemol (25.4), *α*-caryophyllene (12.5%)	3.2	10.9	16.5	68.1	0	0	0	0	Baloch et al. (2025)
CB4	*C. brachycarpa* Vahl ex DC.	Pakistan, Karor Lal Esan fl, October	*γ*-eudesmol (37.0%), elemol (25.0), *α*-caryophyllene (13.1%)	3.2	10.1	17.3	67.7	0	0	0	0	Baloch et al. (2025)
CB5	*C. brachycarpa* Vahl ex DC.	Iran nr, September	Thunbergol (46.1%), *α*-eudesmol (12.7%), elemol (7.5%)	4.3	1.4	4.5	32.3	52.1	0	0.5	1.4	Rassouli et al. (2014)
CB6	*C. brachycarpa* Vahl ex DC.	Iran nr, March	*Ent*-sandaracopimaradien-3*β*-ol (68.0%), cembrene (7.0%), juniper camphor (4.2%)	1.5	1.5	3.3	16.8	75.7	0	0	0	Joukar et al. (2023a)
CCH	*C. chrysantha* Decne.	Egypt fl, nr	1-isocyano-4-methyl benzene (21.7%), *γ*-muurolene (12.5%), *cis*-nerolidole (10.4%)	0.3	0	32.4	12.5	0	0	22.7	0	Hashem and Wahba (2000)
CCO	*C. coluteoides* Boiss.	Iran fl, July	Piperitone (40.4%), decanal (18.7%), elemol (9.2%)	2.7	41.6	4.2	16.4	0	0	0	28.5	Mazloomifar et al. (2003)
CD1	*C. droserifolia* (Forssk.) Delile	Egypt fl, March	*Cis*-nerolidol (37.6%), *α*-cadinol (9.3%), *δ*-cadinene (7.6%)	0	14.4	16.4	45.6	0.3	0.8	3.1	18.9	Abd El-Gawad et al. (2018)
CD2	*C. droserifolia* (Forssk.) Delile	Jordan fl, April	(*E*)-3,7,11-trimethyl-1,6,10-decatrien (11.8%), carotol (10.1%), *δ*-cadinene (8.9%)	0.3	0.3	30.8	43.7	0	1.1	8.9	14.2	Muhaidat et al. (2015)
CF	*C. fimbriata* Vicary	Oman	Present study	13.5	9.8	9.6	12.4	10.1	8.6	30.2	1.8	
CI1	*C. iberica* DC.	Iran nr, June	Carotol (21.8%), germacrene D (15.8%), *β*-cubebene (15.5%)	0.8	0	56.8	34.6	0	7.8	0	0	Mirza et al. (2005)
CI2	*C. iberica* DC.	Iran fr, July	Lavandulyl acetate (26.6%), *p*-cymene (13.7%), geranyl acetate (12.0%)	17.3	55.0	8.2	16.6	0	2.9	0	0	Bamoniri et al. (2009)
CK	*C. khorassanica* Bunge & Bien. ex Boiss.	Iran nr, May	*o*-isopropenyltoluene (46.7%), duodecyclic acid (11.0%), geranyl acetone (6.6%)	0	2.7	20.2	8.1	0.6	12.3	0	51.5	Joukar et al. (2024a)
CM	*C. monophylla* L.	Kenya nr, August	Terpinolene (14.0%), 1-*α*-terpeneol (10.0%), pentacosane (9.0%)	17.0	11.0	9.0	2.0	5.0	0	0	21.0	Ndungu et al. (1995)

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Table 2. (Continued)

Acronym	Taxa	Origin[a]	Essential oils' main compounds	MH	OM	SH	OS	D	AE	ND	O	Reference
CO	*C. oxypetala* Boiss.	Iran fl, April	Sandaracopimaradien-3β-ol (71.9%), cembrene A (7.1%)	0	1.4	4.2	13.4	79.8	0	0	1.2	Doulah et al. (2017)
CP1	*C. pallida* Kotschy	Oman, Al Raka	Present study	8.9	2.5	32.2	24.2	3.2	16.2	0	8.9	
CP2	*C. pallida* Kotschy	Oman, Haima	Present study	10.1	1.7	25.4	33.4	0.5	18.1	0	2.9	
CQ	*C. quinquenervia* DC.	Iran nr, April	β-caryophyllene (29.0%), β-elemene (11.0%), *p*-xylene (4.1)	4.7	1.4	49.3	3.2	0	0	4.9	35.7	Joukar et al. (2023a)
CRA	*C. ramosissima* Parl. ex Webb	Saudi Arabia fl, April	Cubenol (18.2%), 3(*E*)-cembrene (6.1%), methyl hexadecanoate (5.7%)	0	11.2	18.7	35.4	6.1	6.0	1.0	12.6	Al-Humaidia et al. (2019)
CRO	*C. rostrata* Bobrov	Iran fl, June	4-methyl-dodecan-1-ol (14.1%), farnesan (10.5%), 2-methyl-nonane (5.4%)	0	3.2	11.1		6.0	1.1	0	78.2	Joukar et al. (2023b)
CRUP	*C. rupicola* Vicary	Saudi Arabia fl, April	2-methyl isothiocyanate (42.2%), cubenol (20.1%), hexanal (5.6%)	0.1	2.3	7.2	36.5	0.4	1.5	42.3	8.3	Al-Humaidia et al. (2019)
CRUT1	*C. rutidosperma* DC.	Jamaica nr	(*Z*)-phytol (65.1%), *n*-hexadecanol (7.5%), *n*-octadecanol (5.0%)	0	0	0	0	68.0	0.5	0	17.6	McNeil et al. (2018)
CRUT2	*C. serrata* Jacq.	Jamaica nr	(*Z*)-phytol (53.0%), piperonal (11.5%)	0	0	0	0.3	56.4	0	1.3	32.4	McNeil et al. (2012)
CSE	*C. spinosa* Jacq.	Jamaica fl, August	(*Z*)-phytol (31.3%), integerrimine (5.5%), incensole (4.0%)	0	0.9	1.8	3.3	47.7	0.9	0	26.2	McNeil et al. (2010)
CSP	*C. trinervia* Fresen	Jordan fl, April	1,5-hexandien-3-ol (28.3%), santene (20.0%), 3-methyl-2-methylenebutanitrile (14.9%)	21.8	10.6	1.7	0	0	0.7	26.6	34.5	Muhaidat et al. (2015)
CTR	*C. turkmena* Bobrov	Iran pre fl, April	Thymol (30.9%), *m*-thymol (24.0%), cembrene (11.0%)	6.2	62.8	9.0	1.4	11.0	0	8.4	0.1	Joukar et al. (2024b)
CCH	*C. chrysantha* Decne.	Egypt fl, nr	1-isocyano-4-methyl benzene (21.7%), γ-muurolene (12.5%), *cis*-nerolidole (10.4%)	0.3	0	32.4	12.5	0	0	22.7	0	Hashem and Wahba (2000)

Note: [a]Origin = Country of collection, vegetative stage, month of collection; fl = flowering stage; fr = fruiting stage; nr = not reported; **MH** = Monoterpene Hydrocarbons; **OM** = Oxygenated Monoterpenes; **SH** = Sesquiterpene Hydrocarbons; **OS** = Oxygenated Sesquiterpenes; **D** = Diterpenes; **AE** = Organic acids and esters; **ND** = Nitrogen derivatives; **O** = Other compounds; CLWS = cultivated at low water stress; CMWS = cultivated at medium water stress; CHWS = cultivated at high water stress.

of *C. amblyocarpa* (Abd-El-Gawad et al., 2021). The nitrogen derivatives identified in **CF** made this sample highly particular. These derivatives, although structurally different from those of **CF**, have also been found in *C. chrysantha* Decne. (Hashem & Wahba, 2000), in *C. droserifolia* (Muhaidat et al., 2015), and in *C. trinervia* Fresen (Muhaidat et al., 2015), and not in all the *Cleome* specimens' essential oils studied so far. This may suggest that different enzymatic systems may exist in the biosynthesis of these compounds and that it should be investigated to highlight different not only botanical differences between the species.

3.2 HCA and PCA Analysis

To evaluate similarities between the chemical compositions of *Cleome* taxa essential oils, the total relative compositions of the individual chemical classes were taken into consideration (Table 2).

Table 2 reports all aerial parts essential oils obtained by hydrodistillation, the place of origin of each individual sample, the main components (>3%) identified through GC-MS analysis, and the different chemical classes considering the contribution (%) of individual compounds for each individual class. The statistical analyzes were carried out considering only the chemical classes that significant contribution to the total composition of essential oils obtained through hydrodistillation of the aerial parts alone, according to the loading plot obtained by principal component analysis (PCA) and hierarchical cluster analysis (HCA) for monoterpene hydrocarbons (**MH**), oxygenated monoterpenes (**OM**), sesquiterpene hydrocarbons (**SH**), oxygenated sesquiterpenes (**OS**), diterpenes (**D**), organic acids and esters (**AE**), nitrogen derivatives (**ND**), and other compounds (**O**).

The PCA of Cleome taxa revealed that the first and second principal components (PC1 and PC2) represented the 71.3% of the total information (Figure 1). The general structure of the dendrogram (Figure 2) created by HCA indicated

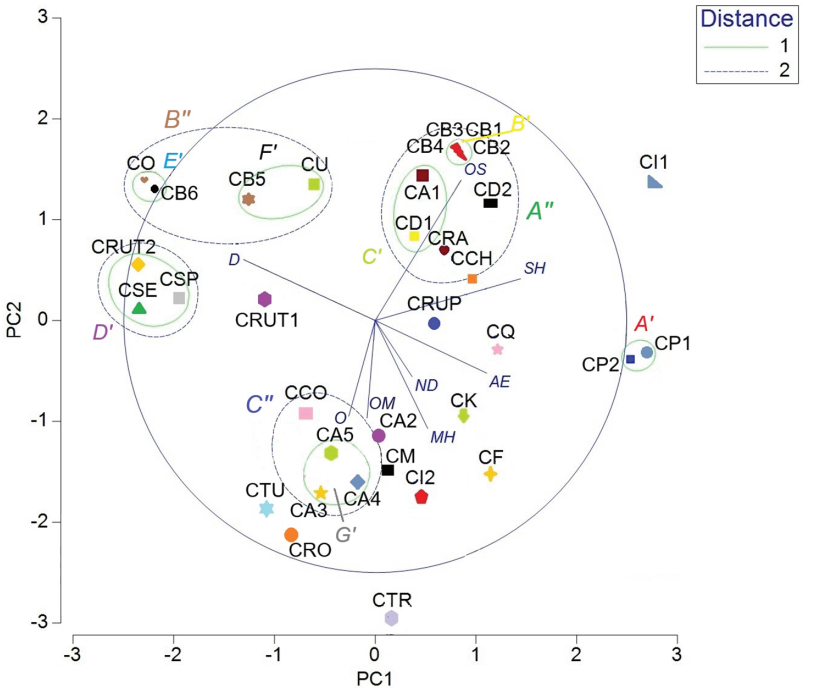

Figure 1. Principal component analysis (PCA) of the essential oil composition of published *Cleome* taxa based on the principal chemical classes of compounds: monoterpene hydrocarbons (**MH**), oxygenated monoterpenes (**OM**), sesquiterpene hydrocarbons (**SH**), oxygenated sesquiterpenes (**OS**), diterpenes (**D**), organic acids and esters (**AE**), nitrogen derivatives (**ND**), and other compounds (**O**). The vectors shown are the eigenvectors of the covariance matrix. The *Cleome* taxa acronym is reported in Table 2

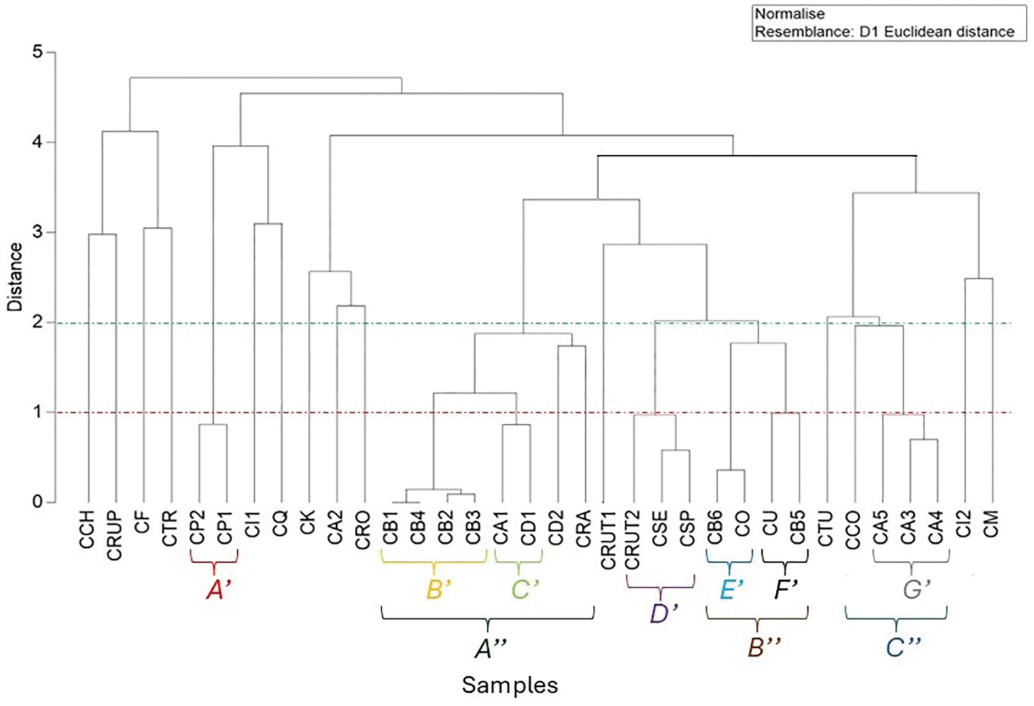

Figure 2. Dendrogram obtained by HCA based on the Euclidian distances with *Cleome* taxa essential oils. The *Cleome* taxa acronym is reported in Table 2

the existence of seven main clusters of populations, based on their chemical composition and on the Euclidean distance between groups (**A′**–**G′**) (distance ≤ 1), and a solution with three clusters (A″, B″ and C″), with a dissimilarity ≤2 (Figure 2) As shown in the loading graph (Figure 1), all variables affected negatively and positively both PC1 and PC2.

In fact, PC1 (42.8%) was represented mainly by **OS**, **SH**, and **D** in the positive score, and with a good **O**, **OM**, **MH**,

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ND, and **AE** contributions in negative scores; meanwhile, PC2 (28.5%) was represented mainly by a clear negative score of **D** and positive scores of **OS**, **SH**, and **AE**.

The graph (Figure 1), in fact, presented a first cluster, group ***B′***, formed by Pakistani *C. brachycarpa* samples (**CB1-CB4**) (Baloch et al., 2025) which were characterized by a high presence of oxygenated sesquiterpenes (66.9–68.1%), medium of **SH** (16.5–17.2%) and **OM** (9.7–10.9%), low presence of **MH** (2.3–3.2%), and the absence of other chemical classes. Cluster ***C′***, formed by **CA1** (Abd-El-Gawad et al., 2021) and **CD1** (Abd El-Gawad et al., 2018) samples, differs from ***B′***, only because the latter samples did not present **MH** derivatives and because they had minimal amounts of **O** compounds (12.3–18.9%, respectively). At this level of similarity (Euclidean distance ≤ 1), clusters ***D′*** and ***G′*** were completely dissimilar. ***G′***, consisting of samples from *C. rutidosperma*, *C. serrata*, and *C. spinosa* samples **(CRUT2, CSE, CSP**, respectively) (Muhaidat et al., 2015; McNeil et al., 2010; McNeil et al., 2012), is influenced by the clear presence of diterpene derivatives (47.7–68.0%) and the medium-high presence of **O** compounds (17.6–32.4%); cluster ***G′***, despite presenting moderate amounts of **O** derivatives, differs from cluster ***D′*** only in the great presence of **OM** compounds (66.1–71.1%). Separate species samples, *C. austroarabica* (**CU**) (Rehman et al., 2021) and *C. brachycarpa* (**CB5**) (Rassouli et al., 2014), instead, formed a separate cluster, ***F′***, influenced by the medium presence of **D** and **OS**, the absence of **AE** class, and the low presence of compounds belonging to the remaining classes. Since these samples (**CB5** and **CU**) were identified as different species, but were characterized by identical compounds (thunbergol, α-eudesmol, and elemol), it would be appropriate to reinvestigated these samples.

The two clusters ***A′*** and ***E′***, formed by the samples **CP1-CP2** and **CO-CB6** (Joukar et al., 2023a; Doulah et al., 2017), and influenced, respectively, the positive and negative scores of PC1, were out of the 95% confidence marked by the blue circle. While samples **CP1** and **CP2** came from extractions performed on the same species (*C. pallida*), it is interesting to note that **CB6** and **CO** essential oils, respectively obtained from Iranian *C. brachycarpa* and Omani *C. austroarabica*, were chemically very similar: high amount of diterpene derivatives (75.7–79.8%), medium amount of **OS** (16.8–13.4%), and low amount of the other classes. Moreover, compositionally, for both species, sandaracopimaradien-3β-ol was the main and majority compound, followed by cembrene derivatives. It would therefore be interesting to investigate, both botanically and genetically, possible correlations between these two species.

By increasing the level of dissimilarity (cut-off level 2) it is possible to identify three macro clusters: ***A″***, ***B″***, and ***C″***. The group ***A″*,** in addition to the aforementioned clusters ***B′*** and ***C′***, it also includes the **CD2** (Muhaidat et al., 2015) and **CRA** (Al-Humaidia et al., 2019) samples. These were not initially included in clusters ***B′-C′*** because they differed in their higher content of **SH**, **D**, and **AE** derivatives, and a lesser influence of **OS** compounds. However, the compositional difference in terms of chemical compounds remains clear.

Cluster ***G′*** could be expanded to this level of similarity to cluster ***C″***, thus statistically including the **CCO** sample, characterized by a greater presence of **OS** and **O** metabolites, unlike the **CA3–CA5** samples. In fact, although **CCO** (Mazloomifar et al., 2003) contains sesquiterpene derivatives such as elemol (9.2%) and β-eudesmol (5.2%), present also in **CA3-CA5** (Shahin et al., 2018), it is differentiated by the clear presence of aldehydes such as decanal and dodecanal; therefore, the clustering at a cut-off of ≤1 is statistically correct.

Finally, a cut-off of 2 would lead to clusters ***E′*** and ***F′*** being grouped into a larger cluster ***B″***, but it has already been noted how these two groups differed at the compositional and elemental level.

The statistical analysis showed clear divergences at the chemical level even between species of the same genus, for example **CB6** (Joukar et al., 2023a) compared to samples **CB1–CB5** (Baloch et al., 2025; Rassouli et al., 2014), but in any case, beyond the small clusters discussed and the uncertainty in identifying some plants, the botanical differentiation of the various *Cleome* species would seem to be chemically correct.

The evidence, however, that emerges from the examination of Table 2, is that some *Cleome* species investigated so far (**CCH, CD2, CF, CRUP, CSP, CTR**) appeared to be richer in isothiocyanate derivatives others that present limited quantities (**CA2, CA3, CU, CB5, CD1, CQ, CRA, CRUT2**) or are completely devoid of them (**CA1, CA4, CA5, CB1-4, CB6, CCO, CI1-2,CK, CM, CO, CP1-2, CRO, CRUT1,** and **CSE**).

4 Conclusions

As a brief overall result, chemical analyzes performed through GC-MS technique were conducted on the Omani essential oils obtained from two accessions of *Cleome pallida* (**CP1**, and **CP2**), different in terms of chemical composition, one with guaiol as the major compound (17.75%, **CP1**), while **CP2** characterized by the significant presence of caryophyllene oxide (19.83%). Instead, *C. fimbriata* (**CF**) essential oil was rich in isothiocyanate derivatives (1-isothiocyanato-3-methylbutanem, 20.7%), a chemical class presented in some investigated *Cleome* ssp. essential oil. Furthermore, statistical studies (PCA and HCA) demonstrated that the *Cleome* species within displayed remarkable biodiversity in terms of chemical compounds. To the extent of the authors' knowledge, this is the first study of its kind to establish the biodiversity of *Cleome* ssp. at a statistical level; therefore, the present study has pioneering value. This is especially true in consideration of the fact that *Cleome* ssp. are spontaneous in many religions of the Earth and only a few specimens of limited areas have been investigated to date.

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Availability of Data and Materials

The authors declare that the data supporting the findings of this study are available within the paper and its Supplementary Information files. Should any raw data files be needed in another format they are available from the corresponding author upon reasonable request. Source data are provided with this paper.

Conflicts of Interest

The authors declare that they have no competing financial interests.

Supporting Information

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