

SUPPLEMENTAL INFORMATION

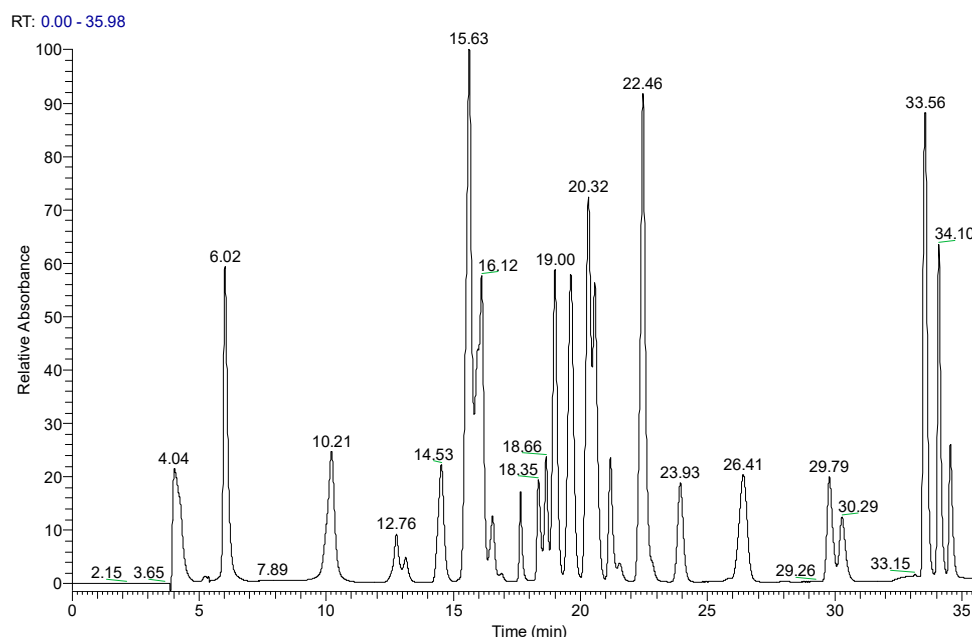
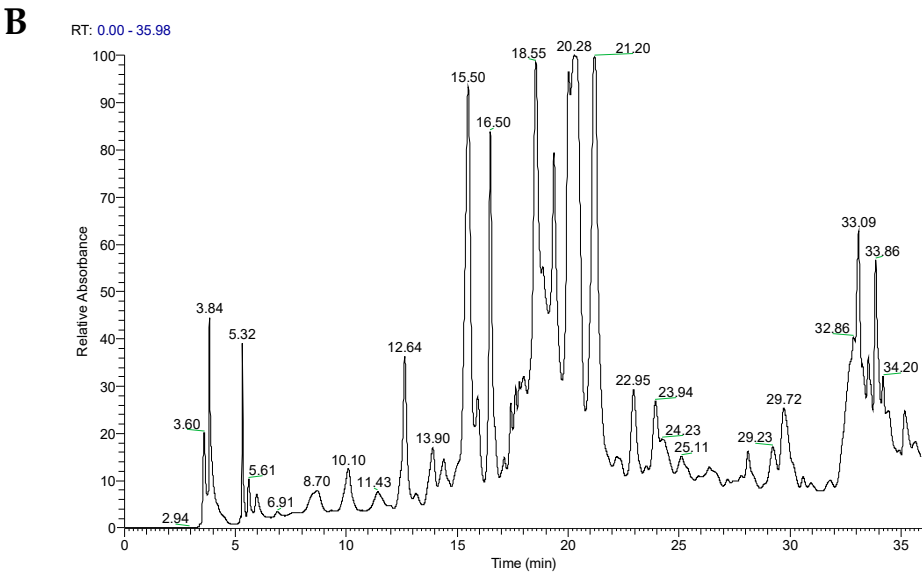
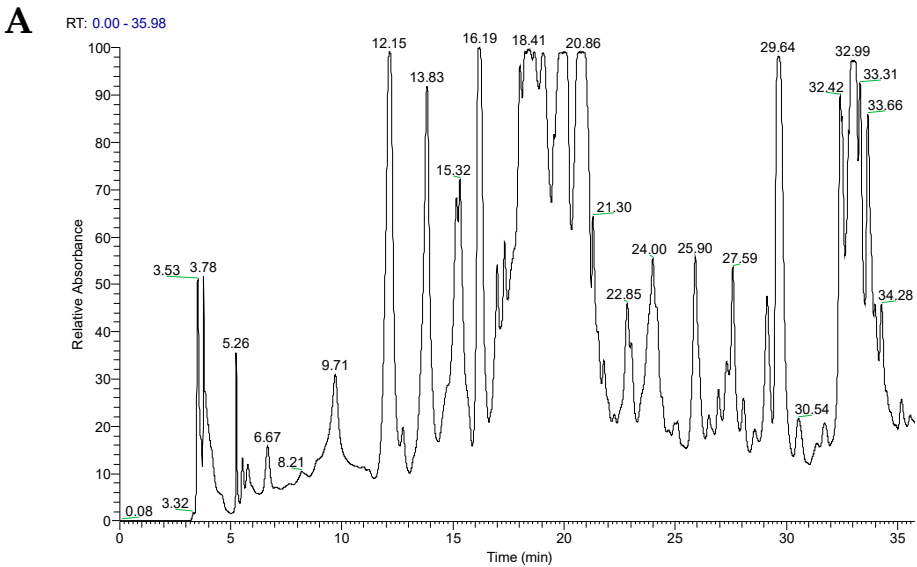


Figure S1. LC–MS chromatogram of standards phenolic compounds in the methanol–water.

Table S1. Standards used to identify and quantify phenolic compounds in *Cladanthus mixtus*.

Peak	Phenolic compound	Retention time (min)	Masse (m/z)	Calibration curve	Coefficient of deter- mination (R2)
1	Gallic acid	6,02	169,43	$Y = 52,23 \cdot X - 127,5$	0,9978
2	Protocatechuic acid	10,21	153,46	$Y = 34,24 \cdot X - 22,30$	0,9994
3	Chlorogenic acid	12,76	353,05	$Y = 9,013 \cdot X - 21,10$	0,9977
4	Catechin	13,13	289,31	$Y = 3,962 \cdot X + 0,5337$	0,9994
5	p-hydroxybenzoïc acid	14,53	137,43	$Y = 24,77 \cdot X - 9,242$	0,9987
6	Caffeic acid	15,63	179,41	$Y = 97,26 \cdot X + 142,7$	0,999
7	Vanillic acid	15,97	167,00	$Y = 29,39 \cdot X + 16,70$	0,9987
8	Syringic acid	16,12	197,00	$Y = 44,26 \cdot X + 26,40$	0,9997
9	Rutin	17,65	609,18	$Y = 8,200 \cdot X - 1,036$	0,999
10	Ellagic acid	18,35	301,22	$Y = 12,18 \cdot X + 54,35$	0,9982
11	Luteolin-7-O-glucoside	18,66	447,00	$Y = 14,78 \cdot X + 3,791$	0,9992
12	p-Coumaric acid	19,00	164,00	$Y = 50,04 \cdot X - 48,94$	0,9986
13	Vanillin	19,63	151,20	$Y = 61,85 \cdot X - 25,55$	0,9984
14	Ferulic acid	20,32	193,00	$Y = 65,81 \cdot X - 93,12$	0,9982
15	Naringin	20,57	579,31	$Y = 47,61 \cdot X - 38,64$	0,9987
16	Apigenin-7-O-glucoside	21,18	431,22	$Y = 17,00 \cdot X - 3,910$	0,9983
17	Rosmarinic acid	22,46	359,10	$Y = 87,94 \cdot X - 5,717$	0,9993
18	Salicylic acid	23,93	137,16	$Y = 19,27 \cdot X + 1,614$	0,9992
19	Methyl paraben	26,41	151,53	$Y = 29,78 \cdot X + 0,7684$	0,9991
20	Luteolin	29,79	285,35	$Y = 20,42 \cdot X - 15,82$	0,9983
21	Quercetin	30,29	301,00	$Y = 13,50 \cdot X - 5,296$	0,999

22	Apigenin	33,56	269,69	$Y = 66,91 \cdot X + 41,21$	0,9993
23	Kaempferol	34,10	285,45	$Y = 38,06 \cdot X - 21,28$	0,9988
24	Isorhamnetin	34,55	315,26	$Y = 15,74 \cdot X + 19,51$	0,9993



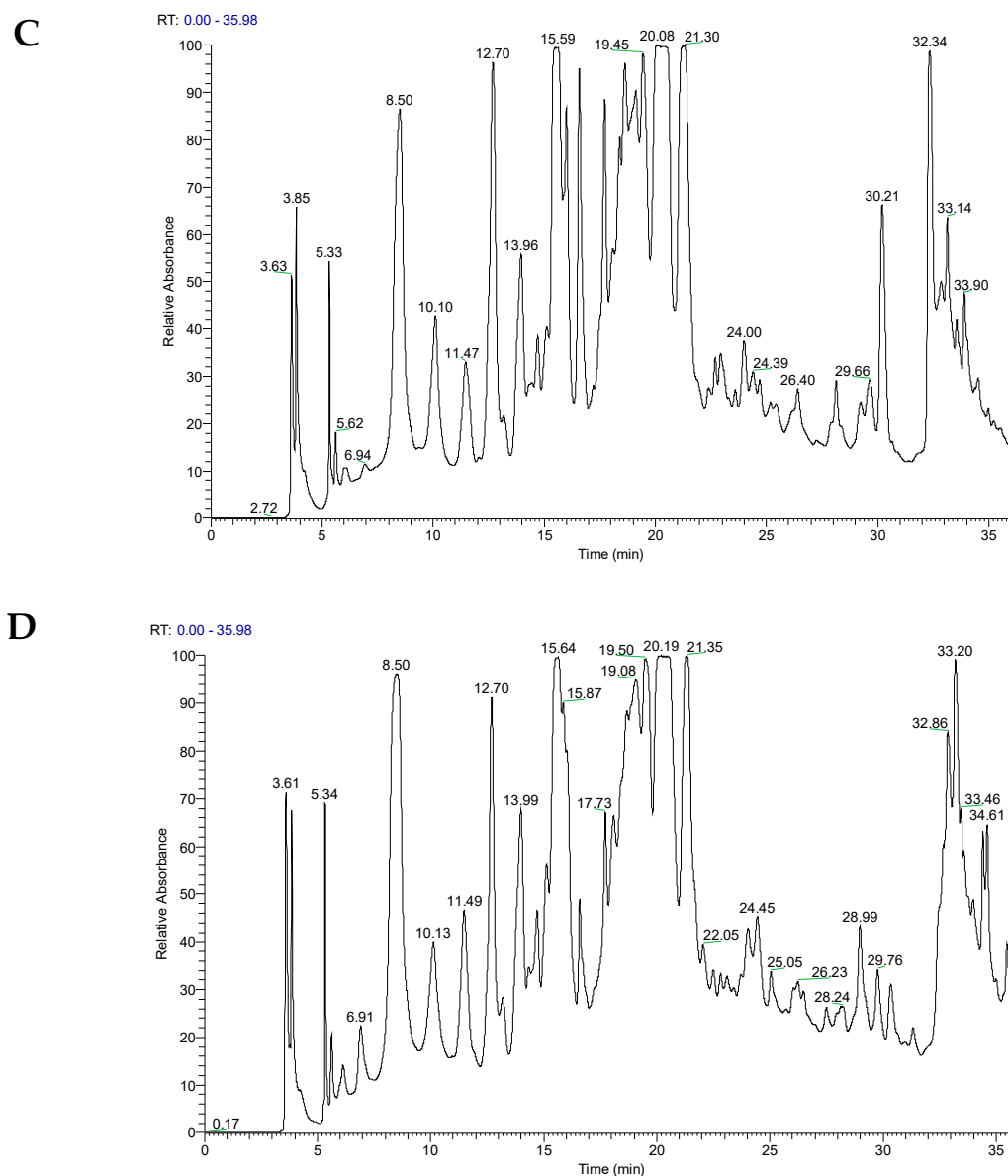


Figure S2. HPLC-MS chromatograms of *Cladanthus mixtus* extracts as detected at 280 nm
(A) flowers, (B) leaves, (C) stems, (D) roots.

Table S2: Chemical composition of terpenoids obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Area (%)			
			Flowers (CM-F)	Leaves (CM-L)	Stems (CM-S)	Roots (CM-R)
β -sitosterol	C ₂₉ H ₅₀ O	414.7	6.25	--	--	--
Lupeol	C ₃₀ H ₅₀ O	426.7	--	14.66	--	8.69
Phytol	C ₂₀ H ₄₀ O	296.5	--	11.39	6.41	0.97
Eucalyptol	C ₁₀ H ₁₈ O	154.2	0.48	3.95	2.83	1.22
Campesterol	C ₂₈ H ₄₈ O	400.7	2.81	1.28	--	--
Taraxasterol	C ₃₀ H ₅₀ O	426.7	0.87	--	--	--

2,6-Octadienal, 2,6-dimethyl-8-(tetrahydro-2H-2-pyran-2-yl-oxo)	C ₁₅ H ₂₄ O ₃	252.3	--	6.88	--	--
Neophytadiene	C ₂₀ H ₃₈	278.5	--	2.16	--	--
Tetradecane, 2,6,10-trimethyl	C ₁₇ H ₃₆	240.5	--	2.38	--	--
Pentadecan-2-one, 6,10,14-trimethyl	C ₁₈ H ₃₆ O	268.5	--	1.93	0.85	--
Isoshyobunone	C ₁₅ H ₂₄ O	220.3	--	1.00	--	--
Caryophyllene oxide	C ₁₅ H ₂₄ O	220.3	--	0.57	--	--
(3 α)-D:A-Friedooleanan-3-ol	C ₃₀ H ₅₂ O	428.7	--	--	1.23	--
Total			10.41	46.20	11.32	10.88

(--) : Not detected

Table S3: Chemical composition of esters obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Area (%)		
				Leaves (CM-L)	Stems (CM-S)	Roots (CM-R)
Palmitic acid β -monoglyceride	C ₁₉ H ₃₈ O ₄	330.5	7.88	6.32	15.66	13.08
Stearic acid β -monoglyceride	C ₂₁ H ₄₂ O ₄	358.6	3.29	3.21	4.00	5.57
Palmitic acid, methyl ester	C ₁₇ H ₃₄ O ₂	270.5	1.02	--	2.33	1.63
Linoleic acid, methyl ester	C ₁₉ H ₃₄ O ₂	294.5	0.92	--	--	--
Oleic acid, methyl ester	C ₁₉ H ₃₆ O ₂	296.4	0.77	--	--	--
l-Norvaline, N-ethoxycarbonyl-, hexadecyl ester	C ₂₄ H ₄₇ NO ₄	413.6	--	--	3.49	--
l-Proline, N-allyloxycarbonyl-, undec-10-enyl ester	C ₂₀ H ₃₃ NO ₄	351.5	--	--	2.98	--
Diisooctyl phthalate	C ₂₄ H ₃₈ O ₄	390.6	--	--	1.65	--
Artemisyl acetate	C ₁₂ H ₂₀ O ₂	196.3	--	2.47	--	--
Phytyl decanoate	C ₃₀ H ₅₈ O ₂	450.8	--	0.82	--	--
Carbonic acid	C ₃ H ₄ O ₃	88.0	--	0.39	--	--
2-Mercapto-2-methyl-propionic acid	C ₄ H ₈ O ₂ S	120.1	--	--	--	1.09
Benzoic acid, 4-butoxy-3-methoxy-perhydro-1-quinoliziny-1-methyl ester	C ₂₂ H ₃₃ NO ₄	375.5	--	--	--	0.54
Total			13.88	13.21	30.11	21.91

(--) : Not detected

Table S4: Chemical composition of alcohols obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Area (%)		
				Leaves (CM-L)	Stems (CM-S)	Roots (CM-R)
Ethyl iso-allocholate	C ₂₆ H ₄₄ O ₅	436.6	--	--	--	23.28
2,3-Dimethyl-3-pentanol	C ₇ H ₁₆ O	116.2	--	--	--	0.87
1-Hexadecanol	C ₁₆ H ₃₄ O	242.4	--	--	--	0.34
Diallyl methyl carbinol	C ₈ H ₁₄ O	126.2	--	5.39	--	--
2-Methyl-Z,Z-3,13-octadecadienol	C ₁₉ H ₃₆ O	280.5	--	1.09	--	--

1-Methylcycloheptanol	C ₈ H ₁₆ O	128.2	--	0.26	--	--
1-Cyclohexanol, 1-[5-hydroxy-4-methyl-2-hexenyl]	C ₁₃ H ₂₄ O ₂	212.3	--	--	3.98	--
5-Azacyclodecanol	C ₉ H ₁₉ NO	157.2	--	--	1.07	--
Total			--	6.74	5.05	24.49

(--) : Not detected

Table S5: Chemical composition of alkanes obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Leaves (CM-L)	Area (%)	
					Stems (CM-S)	Roots (CM-R)
Eicosane	C ₂₀ H ₄₂	282.5	13.46	2.14	1.97	--
Octadecane, 5,14-dibutyl-	C ₂₆ H ₅₄	366.7	0.23	--	--	--
Tetracosane	C ₂₄ H ₅₀	338.7	0.47	--	--	--
3-Methylpentacosane	C ₂₆ H ₅₄	366.7	0.30	--	--	--
9-Octylhexacosane	C ₃₄ H ₇₀	478.9	0.68	--	--	--
Cyclohexane, (1,1-dimethyl-propyl)-	C ₁₁ H ₂₂	154.2	--	0.49	--	--
1,3,5-Trimethyl-2-octadecyl-cyclohexane	C ₂₇ H ₅₄	378.7	--	--	6.17	2.26
6,6-Dimethyl-10-methylene-1-oxa-spiro[4.5]decane	C ₁₂ H ₂₀ O	180.2	--	--	5.57	--
10-Methyleicosane	C ₂₁ H ₄₄	296.6	--	--	2.24	--
11-Decyltetracosane	C ₃₄ H ₇₀	478.9	--	--	2.18	--
Tritetracontane	C ₄₃ H ₈₈	605.2	--	--	--	0.88
Total			15.14	2.63	18.13	3.14

(--) : Not detected

Table S6: Chemical composition of fatty acid obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Leaves (CM-L)	Area (%)	
					Stems (CM-S)	Roots (CM-R)
(Z)-18-Octadec-9-enolide	C ₁₈ H ₃₂ O ₂	280.4	12.69	--	--	--
Palmitic acid	C ₁₆ H ₃₂ O ₂	256.4	9.1	11.39	--	--
γ-Stearolactone	C ₁₈ H ₃₄ O ₂	282.5	3.8	--	--	--
(Z)-13-Docosenamide	C ₂₂ H ₄₃ NO	337.6	1.17	--	6.18	8.23
Capric acid	C ₁₀ H ₂₀ O ₂	172.2	1.1	--	--	--
(E)-3-methoxy-4-nitro-2-butenic acid	C ₅ H ₇ NO ₅	161.1	--	0.49	--	--
Total			27.86	11.88	6.18	8.23

(--) : Not detected

Table S7: Chemical composition of organic acids obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Leaves (CM-L)	Area (%)	
					Stems (CM-S)	Roots (CM-R)
Oxalic acid, dihydrazide	C ₂ H ₆ N ₄ O ₂	118.1	1.88	0.51	2.74	3.47

2,5-Furandione, 3-(2-decenyl)dihydro-	C ₁₄ H ₂₂ O ₃	238.3	0.64	--	--	--
3-Methylbutanoic acid	C ₅ H ₁₀ O ₂	102.1	--	--	--	1.23
1-Propylheptyl ethylphosphonofluoridate	C ₁₂ H ₂₆ FO ₂ P	252.3	--	1.16	--	--
3-Methylcyclopentyl acetate	C ₈ H ₁₄ O ₂	142.2	--	0.18	--	--
Total			3.07	1.85	2.74	4.70

(--) : Not detected

Table S8: Chemical composition of benzene and its derivatives obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Area (%)		
				Leaves (CM-L)	Stems (CM-S)	Roots (CM-R)
1-Nitro-3-(propoxy-methyl)benzene	C ₁₀ H ₁₃ NO ₃	195.2	--	--	--	8.15
Loliolide	C ₁₁ H ₁₆ O ₃	196.2	1.64	3.53	3.28	--
Benzaldehyde, 4-methyl-	C ₈ H ₈ O	120.1	--	--	2.45	--
ethyl 3,4-dihydro-1H-isochromene-1-carboxylate	C ₁₂ H ₁₄ O ₃	206.2	1.21	--	--	--
(3-Nitrophenyl) methanol, 3-methylbutyl ether	C ₁₂ H ₁₇ NO ₃	223.2	--	2.85	--	--
5,5,8a-Trimethyl-3,5,6,7,8,8a-hexahydro-2H-chromene	C ₁₂ H ₂₀ O	180.2	--	1.24	--	--
Total			2.85	7.62	5.73	8.15

(--) : Not detected

Table S9: Chemical composition of phenols obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Area (%)		
				Leaves (CM-L)	Stems (CM-S)	Roots (CM-R)
Vanillin	C ₈ H ₈ O ₃	152.1	--	--	--	4.21
2-Methoxy-4-vinylphenol	C ₉ H ₁₀ O ₂	150.1	--	0.52	--	1.28
Phenol, 2,6-dimethoxy-	C ₈ H ₁₀ O ₃	154.1	--	--	--	0.51
6-O-Acetyl-1-[[4-bromophenyl] sulfonyl]-β-D-glucoside	C ₁₄ H ₁₇ BrO ₈ S	425.2	--	--	1.61	--
4-Hydroxy-2-methylacetophenone	C ₉ H ₁₀ O ₂	150.1	0.41	--	--	--
Total			0.41	0.52	1.61	6.00

(--) : Not detected

Table S10: Chemical composition of ketones obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Area (%)		
				Leaves (CM-L)	Stems (CM-S)	Roots (CM-R)
Cyclobutanone	C ₄ H ₆ O	70.0	--	--	2.89	--
2-Propanone, 1-phenoxy-	C ₉ H ₁₀ O ₂	150.1	--	--	1.58	--
Apocynin	C ₉ H ₁₀ O ₃	166.1	--	--	--	1.03
2',5'-Dimethoxyacetophenone	C ₁₀ H ₁₂ O ₃	180.2	--	--	--	0.64

2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a- trimethyl-, (R)-	C ₁₁ H ₁₆ O ₂	180.2	--	1.25	--	--
Total			--	1.25	4.47	1.67

(--) : Not detected

Table S11: Chemical composition of carbonyls obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Leaves (CM-L)	Area (%)	
					Stems (CM-S)	Roots (CM-R)
5-Ethyl-4-methyl-3-heptanone	C ₁₀ H ₂₀ O	156.2	19.27	--	--	--
4-Heptanol, 4-ethyl-2,6-dimethyl-	C ₁₁ H ₂₄ O	172.3	--	1.34	--	--

(--) : Not detected

Table S12: Chemical composition of amines obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Leaves (CM-L)	Area (%)	
					Stems (CM-S)	Roots (CM-R)
<i>N</i> -Butylcyclohexylamine	C ₁₀ H ₂₁ N	155.2	--	--	6.9	--
9-Octadecenamide, (Z)-	C ₁₈ H ₃₅ NO	281.5	--	1.67	--	--
<i>N</i> -Isobutylideneisobutylamine	C ₈ H ₁₇ N	127.2	--	0.65	--	--
2(Ethylenedioxy)ethylamine, <i>N</i> -methyl- <i>N</i> -[4-(1-pyrrolidinyl)-2-butyryl]-	C ₁₄ H ₂₄ N ₂ O ₂	252.3	--	--	--	0.7
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	C ₆ H ₈ O ₄	144.1	1.62	--	--	--
Total			1.62	2.32	6.9	0.7

(--) : Not detected

Table S13: Chemical composition of pyrrolidines obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flowers (CM-F)	Leaves (CM-L)	Area (%)	
					Stems (CM-S)	Roots (CM-R)
2-Hydroxy-1-(1'-pyrrolidiyl)-1-buten-3-one	C ₈ H ₁₃ NO ₂	155.1	0.56	--	--	0.96
1-Pyrrolidinylacetonitrile	C ₆ H ₁₀ N ₂	110.1	0.18	--	0.74	0.33
1-Propanamine, <i>N,N</i> ,2-trimethyl-2-[(2,2,3-trimethyl-1-pyrrolidinyl)oxy]-, (S)-	C ₁₃ H ₂₈ N ₂ O	228.3	0.23	--	--	--
1-(1'-pyrrolidinyl)-2-propanone	C ₇ H ₁₃ NO	127.1	--	--	0.91	--
Pyrrolidine, <i>N</i> -(3-methyl-3-butenyl)-	C ₉ H ₁₇ N	139.2	--	0.22	1.39	--
Total			0.97	0.22	3.04	1.29

(--) : Not detected

Table S14: Chemical composition of pyrimidines and steroids obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Area (%)			
			Flower	Leaf	Stem	Root
Pyrimidines						
2(1H)-Pyrimidinethione, tetrahydro-1,3-dimethyl-	C ₆ H ₁₂ N ₂ S	144.2	--	--	--	2.07
Steroids						
2-Methylene-5alpha-cholestan-3beta-ol	C ₂₈ H ₄₈ O	400.7	--	2.32	--	--
(--): Not detected						

(--) : Not detected

Table S15: Chemical composition of other molecules obtained by GC-MS.

Molecules	Chemical formula	Molecular weight	Flower	Area (%)		
				Leaf	Stem	Root
5-Piperidin-1-yl-furan-2-carbaldehyde	C ₁₀ H ₁₃ NO ₂	179.2	1.69	--	--	--
5-(4Nitrophenoxy)methyl furan-2-carbaldehyde)	C ₁₂ H ₉ NO ₅	247.2	--	--	--	0.64
2,3-Dihydrobenzofuran	C ₈ H ₈ O	120.1	1.46	--	--	--
2-Methylpentadecane-2-thiol	C ₁₆ H ₃₄ S	258.5	--	0.86	--	--
Triphenylphosphine oxide	C ₁₈ H ₁₅ OP	278.3	--	--	3.43	--
Docosyl octyl ether	C ₃₀ H ₆₂ O	438.8	--	0.62	--	--
Butyl(dimethyl)propoxysilane	C ₉ H ₂₂ OSi	174.3	--	--	1.29	--
Guanine-cytosine	C ₉ H ₁₀ N ₈ O ₂	262.2	--	--	--	1.28
Hygrine	C ₈ H ₁₅ NO	141.2	--	--	--	0.38
Cycloheptane, 1,2-dichloro-, cis-	C ₇ H ₁₂ Cl ₂	167.0	--	--	--	1.07
Heptadecane, 9-hexyl-	C ₂₃ H ₄₈	324.6	--	--	--	2.79
Normephedrone	C ₁₀ H ₁₃ NO	163.2	--	--	--	0.61
Vinyl decanoate	C ₁₂ H ₂₂ O ₂	198.3	--	0.4	--	--
1,5-Heptadiene, 1,5-bis(trimethylsilyl-3-methylene-, 1E,5Z-	C ₇ H ₁₂	96.17	1.37	--	--	--
Total			4.52	1.88	4.72	6.77

(--) : Not detected.