

A four-dimensional separation approach by offline 2D-LC/IM-TOF-MS in combination with database-driven computational peak annotation facilitating the in-depth characterization of the multicomponents from *Atractylodes Macrocephalae Rhizoma* (*Atractylodes macrocephala*)

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Asterisk equations used for orthogonality evaluation

$$t_{R,\text{norm}(i)} = \frac{t_I - t_D}{t_G - t_D} \quad (1)$$

$$SZ_- = \sigma \{ {}^1t_{R,\text{norm}(i)} - {}^2t_{R,\text{norm}(i)} \} \quad (2)$$

$$SZ_+ = \sigma \{ {}^2t_{R,\text{norm}(i)} - (1 - {}^1t_{R,\text{norm}(i)}) \} \quad (3)$$

$$SZ_1 = \sigma \{ {}^1t_{R,\text{norm}(i)} - 0.5 \} \quad (4)$$

$$SZ_2 = \sigma \{ {}^2t_{R,\text{norm}(i)} - 0.5 \} \quad (5)$$

$$Z_- = |1 - 2.5|SZ_- - 0.4| \quad (6)$$

$$Z_+ = |1 - 2.5|SZ_+ - 0.4| \quad (7)$$

$$Z_1 = 1 - |2.5 \cdot SZ_1 \cdot \sqrt{2} - 1| \quad (8)$$

$$Z_2 = 1 - |2.5 \cdot SZ_2 \cdot \sqrt{2} - 1| \quad (9)$$

$$A_0 = \sqrt{Z_- \cdot Z_+ \cdot Z_1 \cdot Z_2} \quad (10)$$

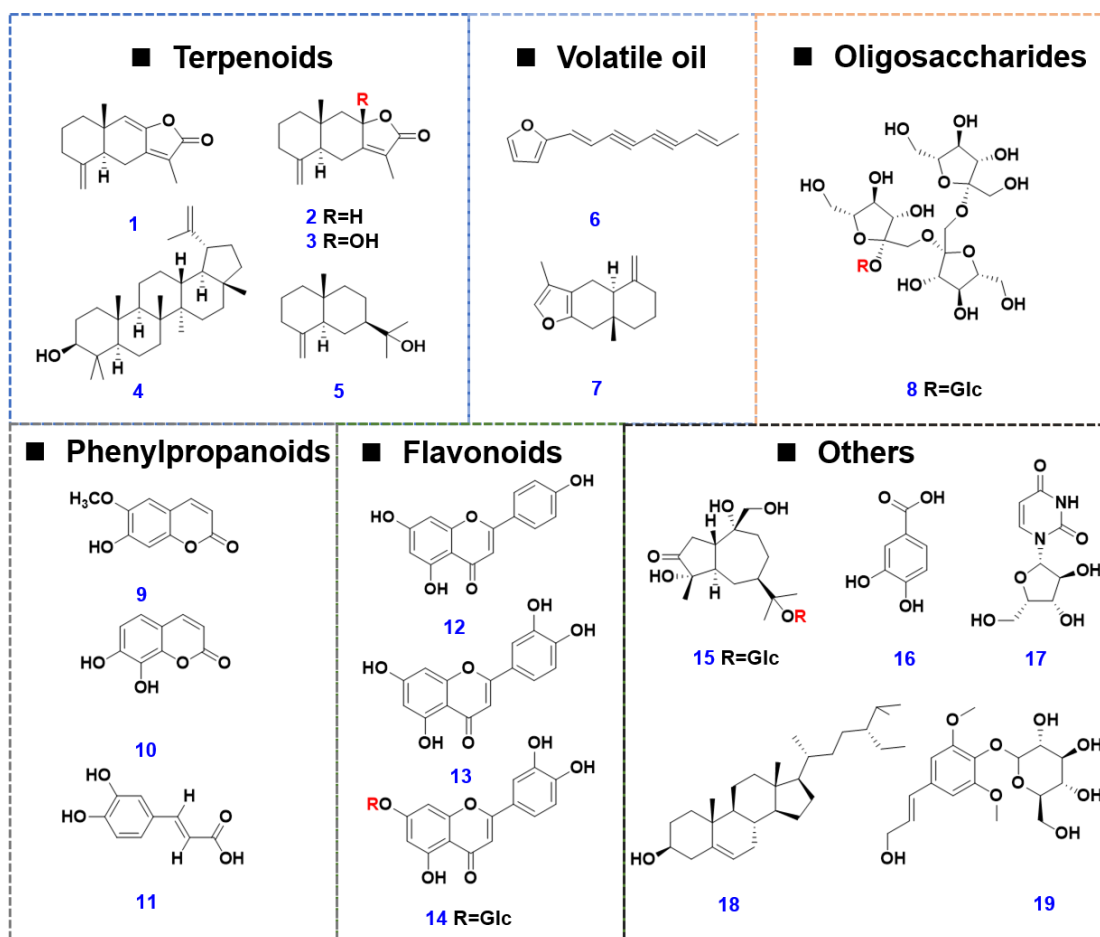


Fig. S1 Chemical structures of 19 reference compounds used in the current work.

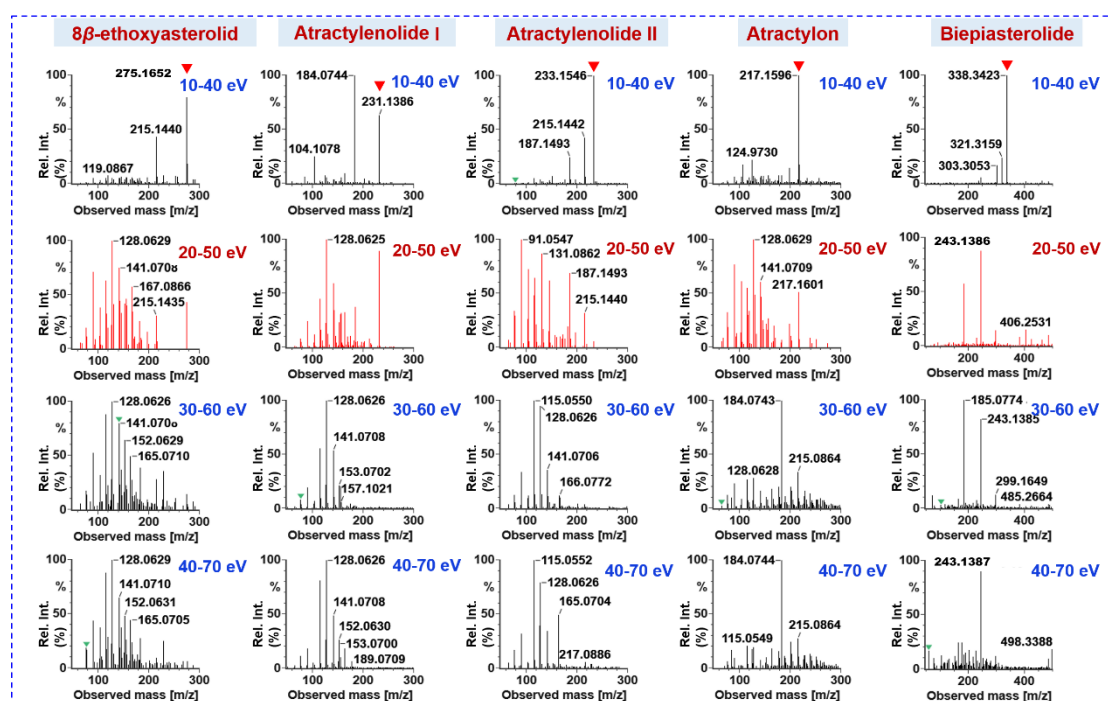


Fig. S2 Optimization of ramp collision energy (RCE) of the Vion IM-QTOF mass spectrometer in the positive mode using five compounds.

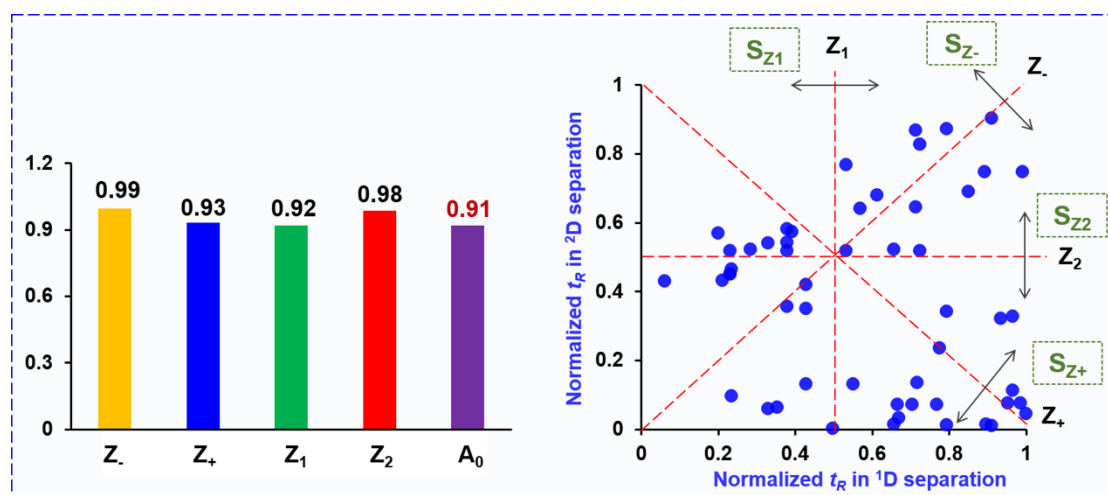


Fig. S3 Orthogonality evaluation of the established offline 2D-LC/IM-QTOF-MS system using the asterisk equations, by calculating the distribution of 54 components based on their relative retention time.

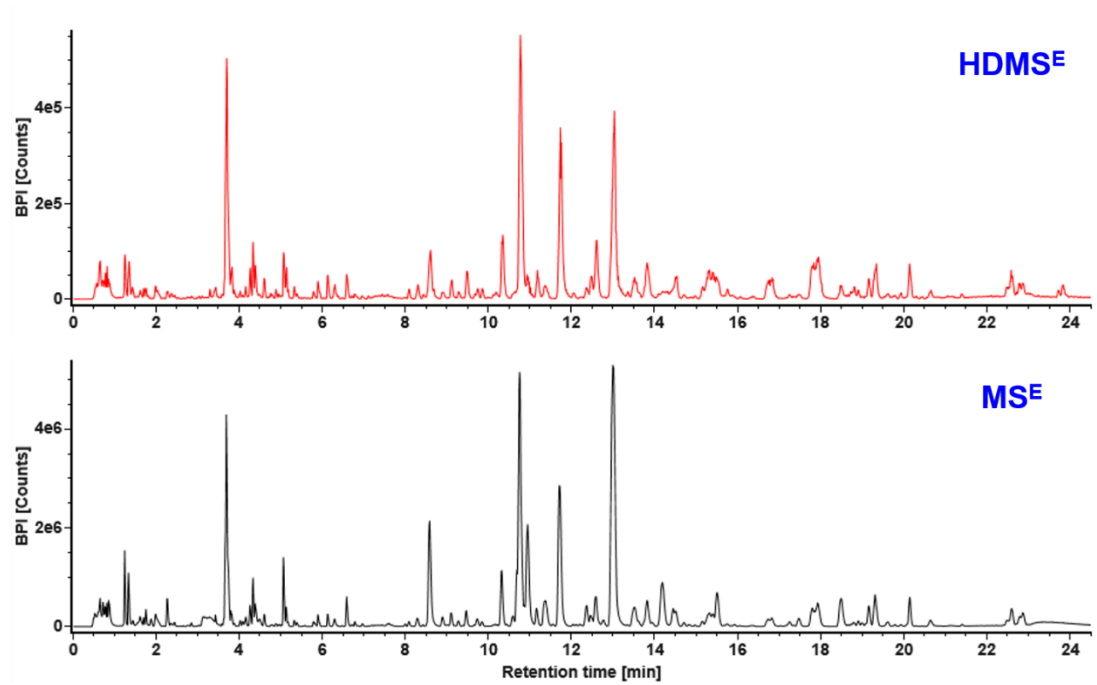


Fig. S4 Comparison of base peak intensity (BPI) chromatograms of the *A. macrocephala* extract by IM-separation enabled HDMS^E and IM-disabled MS^E.

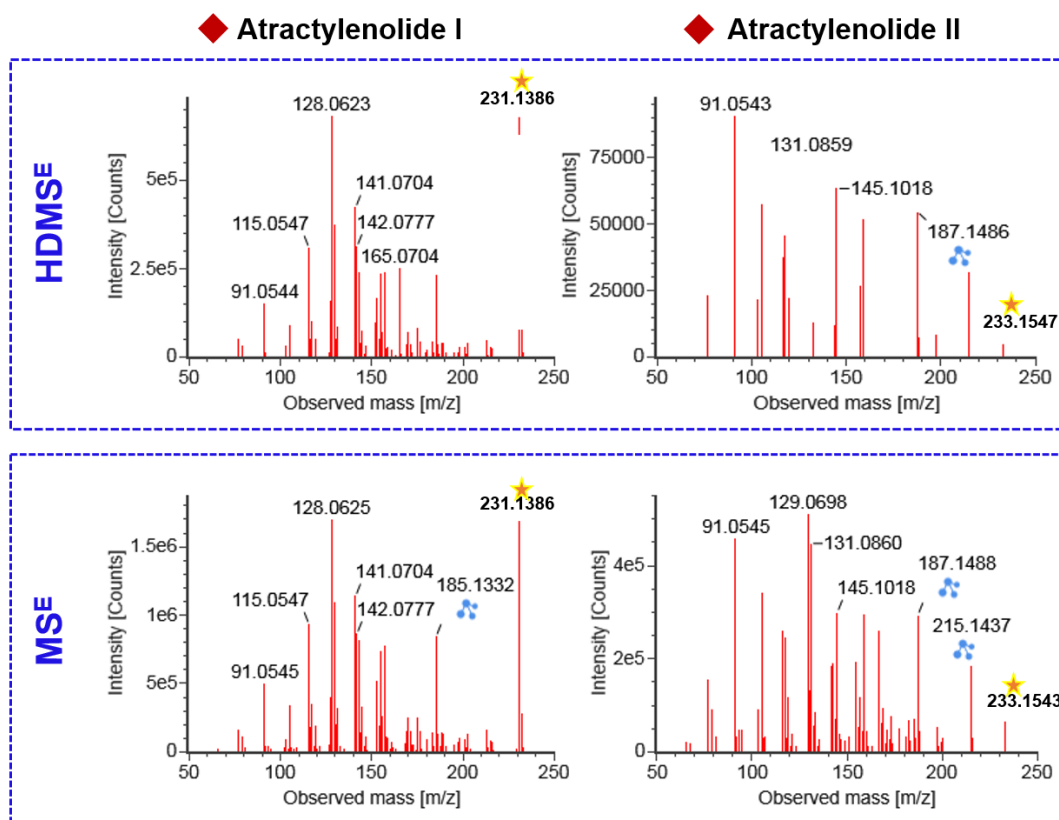


Fig. S5 Comparison of the CID-MS² spectra of two representative reference compounds obtained by IM-separation enabled HDMS^E and IM-disabled MS^E.

Table S1 Detailed information regarding 19 reference compounds used in this work.

No.	Trivial name	M.F.	Exact Mass	Type
1	atractylenolide I	C ₁₅ H ₁₈ O ₂	230.1307	
2	atractylenolide II	C ₁₅ H ₂₀ O ₂	232.1463	
3	atractylenolide III	C ₁₅ H ₂₀ O ₃	248.1412	Terpenoids
4	lupeol	C ₃₀ H ₅₀ O	426.3862	
5	<i>β</i> -cineole	C ₁₅ H ₂₆ O	222.1984	
6	atractylodin	C ₁₃ H ₁₀ O	182.0732	Volatile oil
7	atractylon	C ₁₅ H ₂₀ O	216.1514	
8	nystose	C ₂₄ H ₄₂ O ₂₁	666.2219	Oligosaccharides
9	scopoletin	C ₁₀ H ₈ O ₄	192.0423	
10	patriarchal ephedrine	C ₉ H ₆ O ₄	178.0266	Phenylpropanoids
11	caffeic acid	C ₉ H ₈ O ₄	180.0423	
12	apigenin	C ₁₅ H ₁₀ O ₅	270.0528	
13	luteolin	C ₁₅ H ₁₀ O ₆	286.0477	Flavonoids
14	luteoloside	C ₂₁ H ₂₀ O ₁₁	448.1006	
15	atractyloside A	C ₂₁ H ₃₆ O ₁₀	448.2308	
16	uridine	C ₉ H ₁₂ N ₂ O ₆	244.0695	
17	3,4-dihydroxybenzoic acid	C ₇ H ₆ O ₄	154.0266	Others
18	<i>β</i> -sitosterol	C ₂₉ H ₅₂ O	414.3862	
19	syringin	C ₁₇ H ₂₄ O ₉	372.1420	

Table S2 The in-house library of *Atractylodes macrocephala*.

No.	Name	Formula	M.W.
1	atractylenolide I	C ₁₅ H ₁₈ O ₂	230.1307
2	atractylenolide II	C ₁₅ H ₂₀ O ₂	232.1463
3	atractylenolide III	C ₁₅ H ₂₀ O ₃	248.1412
4	atractylenolide IV	C ₁₇ H ₂₂ O ₅	306.1647
5	atractylenolide V	C ₁₅ H ₂₀ O ₄	264.1362
6	atractylenolide VI	C ₁₅ H ₂₂	202.1722
7	atractylenolide VII	C ₁₇ H ₂₆ O ₂	262.1933
8	3 β -acetoxyl atractylenolide I	C ₁₈ H ₂₄ O ₁₀	304.1675
9	13-hydroxyl-atractylenolide II	C ₁₅ H ₂₀ O ₃	248.1412
10	4-ketone-atractylenolide III	C ₁₅ H ₂₀ O ₃	248.1412
11	eudesm-4(15)-ene-7 β ,11-diol	C ₁₅ H ₂₆ O ₂	238.1933
12	8 β -methoxyatractylenolide	C ₁₆ H ₂₂ O ₃	262.1569
13	atractylenother	C ₁₅ H ₂₁ O ₂	233.1542
14	8-epiatractylenolide III	C ₁₅ H ₂₀ O ₃	248.1256
15	4(<i>R</i>),15-epoxy-8 β -hydroxyatractylenolide II	C ₁₅ H ₈ O ₄	264.1362
16	atractylenolactam	C ₁₅ H ₁₉ NO	229.1467
17	8 β -ethoxyasterolid	C ₁₇ H ₂₃ O ₃	275.1647
18	selina-4(15),7(11)-dien-8-one	C ₁₅ H ₂₁ O	217.1592
19	juniper camphor	C ₁₅ H ₂₅ O	221.1905
20	eudesm-4(15),7-diene-9 α ,11-diol	C ₁₃ H ₂₀ O ₂	208.1463
21	Atractylon	C ₁₅ H ₂₀ O	216.1514
22	atractylmacrols A	C ₁₄ H ₂₄ O	208.1827
23	atractylmacrols B	C ₁₆ H ₂₆ O ₂	250.1933
24	atractylmacrols C	C ₁₈ H ₂₈ O ₃	292.2038
25	atractylmacrols D	C ₁₅ H ₂₂ O	218.1671
26	atractylmacrols E	C ₁₅ H ₂₄ O	220.1827
27	biatractylenolide	C ₃₀ H ₃₈ O ₄	462.2770
28	biatractylenolide II	C ₃₄ H ₄₂ O ₈	578.2880
29	biepiasterolide	C ₃₀ H ₃₈ O ₄	462.2770
30	taraxeryl acetate	C ₃₂ H ₅₂ O ₂	468.3967
31	lupeol	C ₃₀ H ₅₀ O	426.3862
32	14-seneciolyloxytetradeca-2 <i>E</i> ,8 <i>Z</i> ,10 <i>E</i> -trien-4,6-diyne-1-ol	C ₁₉ H ₂₂ O ₃	298.1569
33	14 β -methylbutyryltetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyne-1-ol	C ₁₉ H ₂₄ O ₃	300.1725
34	12-seneciolyloxytetradeca-2 <i>E</i> ,8 <i>Z</i> ,10 <i>E</i> -trien-4,6-diyne-1,14-diacetate	C ₂₃ H ₂₆ O ₆	398.1729
35	12 α -methylbutyryltetradeca-2 <i>E</i> ,8 <i>Z</i> ,10 <i>E</i> -trien-4,6-diyne-1,14-diacetate	C ₂₃ H ₂₈ O ₆	400.1886
36	12-seneciolyloxytetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyne-1,14-diacetate	C ₂₃ H ₂₆ O ₆	398.1729

37	14-acetoxy-12-methylpropionyltetradeca-2 <i>E</i> ,8 <i>Z</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₂₀ H ₂₄ O ₅	344.1624
38	14-acetoxy-12-methylpropionyltetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₂₀ H ₂₄ O ₅	344.1624
39	14-acetoxy-12-seneciolyloxytetradeca-2 <i>E</i> ,8 <i>Z</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₂₁ H ₂₄ O ₅	356.1624
40	14-acetoxy-12 <i>α</i> -methylbutyryltetradeca-2 <i>E</i> ,8 <i>Z</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₂₁ H ₂₆ O ₅	358.1780
41	14-acetoxy-12-seneciolyloxytetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₂₁ H ₂₄ O ₅	356.1624
42	14-acetoxy-12 <i>α</i> -methylbutyryltetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₂₁ H ₂₆ O ₅	358.1780
43	14-acetoxy-12 <i>β</i> -methylbutyryltetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₂₁ H ₂₆ O ₅	358.1780
44	14 <i>α</i> -methylbutyryltetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₁₉ H ₂₄ O ₄	316.1675
45	14 <i>β</i> -methylbutyryltetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₁₉ H ₂₄ O ₄	316.1675
46	12-seneciolyloxytetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₁₉ H ₂₂ O ₄	314.1518
47	12-seneciolyloxytetradeca-2 <i>E</i> ,8 <i>Z</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₁₉ H ₂₂ O ₄	314.1518
48	12-hydroxytetradeca-2 <i>E</i> ,8 <i>Z</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₁₄ H ₁₆ O ₃	232.1099
49	12-hydroxytetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₁₄ H ₁₆ O ₃	232.1099
50	14-acetoxytetradeca-2 <i>E</i> ,8 <i>E</i> ,10 <i>E</i> -trien-4,6-diyn-1-ol	C ₁₆ H ₁₈ O ₄	274.1205
51	4-methoxycinnamic acid	C ₁₀ H ₁₀ O ₃	178.0630
52	caffeic acid	C ₉ H ₈ O ₄	180.0423
53	ferulic acid	C ₁₀ H ₁₀ O ₄	194.0579
54	5-hydroxy ferulic acid	C ₁₀ H ₁₀ O ₅	210.0528
55	2-hydroxy ferulic acid	C ₁₀ H ₁₀ O ₅	210.0528
56	3-hydroxy-1-(4-hydroxy-3-methoxyphenyl) propan-1-one	C ₁₀ H ₁₂ O ₄	196.0736
57	Z-methyl caffeate	C ₁₀ H ₁₀ O ₄	194.0579
58	ethyl 3,4-dihydroxycinnamate	C ₁₁ H ₁₂ O ₄	208.0736
59	scopoletin	C ₁₀ H ₉ O ₄	192.0423
60	7-hydroxycoumarin	C ₉ H ₆ O ₃	162.0317
61	apigenin	C ₁₅ H ₁₀ O ₅	270.0528
62	luteolin	C ₁₆ H ₁₂ O ₅	284.0685
63	scutellarein 6- <i>O</i> -glucoside	C ₂₁ H ₂₂ O ₁₁	450.1162
64	6 <i>β</i> -D-glucopyranosyloxy-5-hydroxy-7-methoxy-flavonone	C ₂₂ H ₂₄ O ₁₀	448.1469
65	8 <i>β</i> -D-glucopyranosyloxy-4',5,7-trihydroxy-flavone	C ₂₁ H ₂₀ O ₁₁	448.1006
66	stereolensin	C ₂₁ H ₂₂ O ₁₂	466.1111
67	stereolensin-4'-trans-caffeate	C ₃₀ H ₂₈ O ₁₄	612.1479

68	β -Sitosterol	C ₂₉ H ₅₀ O	414.3862
69	stigmasterol	C ₂₉ H ₄₈ O	412.3705
70	2-[(2E)-3,7-dimethyl-2,6-octadienyl]-6-methyl-2,5-cyclohexadiene-1,4-dione	C ₁₈ H ₂₄ O	256.1827
71	2,6-dimethoxyquinone	C ₈ H ₈ O ₄	168.0423
72	dictamnocide A	C ₂₁ H ₃₆ O ₉	432.2359
73	syringin	C ₁₇ H ₂₄ O ₉	372.1420
74	uridine	C ₉ H ₁₂ N ₂ O ₆	244.0695
75	atractyloside A	C ₂₀ H ₃₄ O ₁₀	434.2152
76	protocatechuic acid	C ₇ H ₆ O ₄	154.0266
77	palmitic acid	C ₁₆ H ₃₂ O ₂	256.2402
78	2,6-dimethoxyphenol	C ₈ H ₁₀ O ₃	154.0630
79	D-mannitol	C ₆ H ₁₄ O ₆	182.0790

Table S3 Intra-day precision of 2D system ($n=6$).

t_R (min)	1D -Peak Area						Intra-day Precision (%)
2.75	226.65	231.07	243.80	233.60	223.50	242.50	3.22
5.94	2305.85	2254.88	2239.87	2286.28	2254.27	2261.05	0.98
6.78	428.40	437.72	451.90	437.20	440.60	435.90	1.60
10.15	2599.98	2523.70	2554.30	2570.4	2587.40	2594.60	1.03
11.40	1339.10	1293.10	1294.00	1283.00	1292.10	1286.70	1.45

t_R (min)	m/z	Compound	2D -Peak Area						Intra-day Precision (%)
4.26	163.0396	7-hydroxycoumarin	230606	228829	251458	246519	240231	230315	3.00
4.59	193.0502	scopoletin	314527	304171	308149	308745	309689	310967	3.66
7.27	249.1492	atractylenolide III	103540	110247	107048	98291	111461	98338	1.01
13.42	231.1385	atractylenolide I	4312990	4358008	4240761	4131055	4137949	3982109	5.00
21.55	463.2852	biatractylenolide	580921	599089	583561	574492	551391	549408	3.09

Table S4 Inter-day precision of 2D system ($n=3$).

		1D-Peak Area									
t_R (min)		1 Day		2 Day		3 Day		Inter-day Precision (%)			
2.75	276.17	232.60	274.58	268.00	278.95	263.19	257.26	274.09	266.13	5.03	
5.94	2168.22	2120.97	2215.82	2172.46	2263.89	2342.07	2288.97	2390.67	2393.71	4.16	
6.78	415.30	413.00	409.90	432.80	425.60	426.80	402.30	405.50	417.10	2.31	
10.15	2713.75	2855.50	2825.60	2685.00	2725.30	2754.10	2741.00	2713.50	2727.65	1.91	
11.40	1654.51	1625.86	1514.30	1503.10	1480.80	1513.70	1456.60	1436.20	1439.88	4.84	

t_R (min)	m/z	Compound	1 Day		2 Day		3 Day		Inter-day Precision (%)			
4.26	163.0396	7-hydroxycoumarin	243888	247113	265207	322779	357322	350934	293739	298912	298758	13.03
7.27	249.1492	atractylenolide III	113872	102445	93903	100929	110834	108397	103984	105577	105342	3.82
13.42	231.1385	atractylenolide I	3879941	3676717	3897320	4733498	4622094	3883677	3560165	3593775	3531826	11.37
18.72	203.1798	atractylenolide VI	235009	248910	260497	214235	219307	187350	243843	206625	213697	8.67
21.55	463.2852	biatractylenolide	565827	513649	569169	567084	602031	574869	581254	595249	605557	4.77

Table S5 Repeatability of the 2D system ($n=6$).

t_R (min)	m/z	Compound	2D -Pear Area						Repeatability (%)
4.26	163.0396	7-hydroxycoumarin	181148	176378	173398	163691	156273	144406	7.61
5.85	287.0548	luteolin	256440	310863	380230	357169	367092	367195	12.72
6.55	271.0610	apigenin	124328	123768	128226	114205	119713	113775	4.41
7.28	249.1492	atractylenolide III	436641	393857	394607	391266	359476	359615	6.69
13.44	231.1385	atractylenolide I	10385079	10026992	9754072	10029764	10127722	10193616	1.90
21.55	463.2852	biatractylenolide	4427202	4103302	4245030	4198787	4061204	4153541	2.83

Table S6 Detailed information of the 251 components characterized from *Atractylodes macrocephala*.

No.	Observed t_R (min)	M.F.	Observed m/z	Mass error (ppm)	Observed CCS (\AA^2)	MS ² fragments	Identification	Fraction	Structure class	InChI key
1	0.66	C ₁₉ H ₂₂ O ₄	315.1573	-5.7	172.65	244.1178,214.1021,180.1025,	12-seneciolyloxytetradeca-trien-4,6-diyne-1-ol or its isomer	6	Polyacetylene	UJHAKGDWVZI MIT- ADDDGJNWSA- N
2	0.67	C ₁₉ H ₂₂ O ₃	299.1646	1.4	170.16	244.1178,214.1021,180.1025	14-seneciolyloxytetradeca-trien-4,6-diyne-1-ol or its isomer	6	Polyacetylene	XDSKMYLDYJ PBI- JHTNEVNSSA-N
3	0.68	C ₂₁ H ₂₆ O ₅	359.1834	-5.3	179.52	342.1556,262.1299,216.1235,198.1127,180.1025,147.0924	14-acetoxy-12-methylbutyryltetradeca-trien-4,6-diyne-1-ol or its isomer	6	Polyacetylene	WJQQGLCBGRP HBP- AUVZEIHSAN
4	0.7	C ₂₀ H ₃₄ O ₁₀	435.2248	5.3	201.59	395.2219,348.1626,290.1389,216.1196	atractyloside A or isomer	6	Others	TTWARFJENFIGJ K-DNGRJINJSAN
5	0.73	C ₁₇ H ₂₃ O ₃	276.1724	1.5	141.66	220.1102,201.0988,178.0994	ethoxyasterolid or its isomer	8	Sesquiterpenoid	AUEGJURIRHQA IF-XKQJLSEDSAN
6	0.74	C ₂₁ H ₂₆ O ₅	359.1877	6.7	180.3	312.1453,216.1235,187.0881,167.0699	14-acetoxy-12-methylbutyryltetradeca-trien-4,6-diyne-1-ol or its isomer	6	Polyacetylene	WJQQGLCBGRP HBP- AUVZEIHSAN
7	0.76	C ₃₄ H ₄₂ O ₈	579.2957	0.8	231.12	438.2103,388.1849,211.077,104.1075	biatractylenolide II or its isomer	7	Sesquiterpenoid	DJINKBUXGFQI CR- GJDTUZTCSAN

8	0.8	C ₂₁ H ₃₆ O ₉	433.2411	1	155.94	334.1542,277.1391,222.1 239,166.0870,130.0984,1 10.0721	dictamnocide A or its isomer	8	Others	HYCSHXRCGZLJ NW- FPOJDZHTSA-N YVBOVXWVUL
9	0.8	C ₂₃ H ₂₈ O ₆	401.1977	4.6	153.56	240.1311,226.1206,185.0 927,166.0870,142.0864,1 30.0983,110.0720	12-methylbutyryltetradeca- trien-4,6-diyne-1,14-diacetate or its isomer	8	Polyacetylene	MJDC- NLCRFJRRSA-N RLOXIGRNKNT
10	0.8	C ₂₀ H ₂₄ O ₅	345.167	-7.7	176.89	327.1655,285.1169,202.1 003,189.1037	14-acetoxy-12- methylpropionyltetradeca-trien- 4,6-diyne-1-ol or its isomer	7	Polyacetylene	VJQ- JPSRSCNUSA-N TTWARFJENFIGJ
11	0.85	C ₂₀ H ₃₄ O ₁₀	435.2209	-3.6	201.12	435.1849,404.2022,317.1 503,306.1334,238.1200,2 06.1202,150.0919	atractyloside A or isomer	3	Others	K-DNGRJINJSA- N WJQQGLCBGRP
12	0.85	C ₂₁ H ₂₆ O ₅	359.1873	5.5	186.38	306.1278,227.0825,178.1 240,158.0982	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyne-1-ol or its isomer	4	Polyacetylene	HBP- AUVZEZHSA-N RBJDJJGMGHKQ
13	0.86	C ₃₀ H ₃₈ O ₄	463.2844	0.3	212.83	366.2762,330.1548,292.1 506,231.1121,213.1020,1 86.1130	biatractylenolide/biepiasterolide or isomer	3	Sesquiterpeno id	MI- CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N RLOXIGRNKNT
14	0.86	C ₂₀ H ₂₄ O ₅	345.1694	-0.7	186.17	283.1382,240.1227,160.0 760	14-acetoxy-12- methylpropionyltetradeca-trien- 4,6-diyne-1-ol or its isomer	6	Polyacetylene	VJQ- JPSRSCNUSA-N

15	0.87	C ₁₇ H ₂₃ O ₃	276.1719	-0.5	169.24	262.1203,237.1238,230.0 887,148.0749	ethoxyasterolid or its isomer	5	Sesquiterpenoid	AUEGJURIRHQA IF-XKQJLSEDSAN XXTGIQBNHTYL
16	0.87	C ₂₁ H ₂₂ O ₁₁	451.1239	0.9	193.74	289.1406,166.0867,120.0 811,106.0660,91.0548	scutellarein -O-glucoside	5	Flavonoid	OS- GFFZVHSVSA-N BVSZAUUZUUR
17	0.87	C ₂₃ H ₂₆ O ₆	399.1774	-7	191.26	227.0825,216.1255,176.0 454,158.0982	12-seneciolyxotetradeca-trien- 4,6-diyne-1,14-diacetate or its isomer	4	Polyacetylene	PHD- AUVZEZHSA-N WJQQGLCBGRP
18	0.87	C ₂₁ H ₂₆ O ₅	359.1832	-6	192.37	331.1625,283.1389,240.1 227,178.0855,161.1086	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyne-1-ol or its isomer	6	Polyacetylene	HBP- AUVZEZHSA-N YVBOVXWVUL
19	0.88	C ₂₃ H ₂₈ O ₆	401.1938	-5.2	189.04	283.1404,248.1038,178.0 872,174.0914,160.0763	12-methylbutyryltetradeca- trien-4,6-diyne-1,14-diacetate or its isomer	5	Polyacetylene	MJDC- NLCRFJRSA-N WJQQGLCBGRP
20	0.89	C ₂₁ H ₂₆ O ₅	359.1842	-3	177.66	259.1416,245.1263,198.1 106,130.0989	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyne-1-ol or its isomer	7	Polyacetylene	HBP- AUVZEZHSA-N RLOXIGRNKNT
21	1.37	C ₂₀ H ₂₄ O ₅	345.1687	-2.8	193.31	317.1606,256.1297,250.1 452	14-acetoxy-12- methylpropionyltetradeca-trien- 4,6-diyne-1-ol or its isomer	6	Polyacetylene	VJQ- JPSRSCNUSA-N OSOQCOKGODM
22	1.39	C ₁₆ H ₁₈ O ₄	275.1261	-6.2	160.14	178.0869,132.0811,118.0 650,117.0581,115.0545	14-acetoxytetradeca-trien-4,6- diyne-1-ol or its isomer	5	Polyacetylene	ZLC- HJHGKILDSA-N

23	1.6	C ₁₉ H ₂₄ O ₄	317.1753	1.8	176.26	180.0825,119.0493,107.0 494,91.0543	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol	6	Polyacetylene	FPLZCZIWZSNU DH- JPSRSCNUSA-N BVSZAUUZUUR
24	1.73	C ₂₃ H ₂₆ O ₆	399.1811	2.2	194.85	296.1001,258.1354,230.1 386,152.0568	12-seneciolyxytetradeca-trien- 4,6-diyne-1,14-diacetate or its isomer	6	Polyacetylene	PHD- AUVZEZIHSA-N YVBOVXWVUL
25	1.85	C ₂₃ H ₂₈ O ₆	401.1988	7.3	196.11	296.0995,229.1322,166.0 990,152.0568	12-methylbutyryltetradeca- trien-4,6-diyne-1,14-diacetate or its isomer	6	Polyacetylene	MJDC- NLCRFJRSA-N
26	2.13	C ₁₅ H ₂₀ O ₂	233.1541	2.3	224.74	215.1433,205.1593,191.1 436,187.1491,159.0799,1 31.0856	isomer of atractylenolide II	7	Sesquiterpeno id	-
27	2.2	C ₉ H ₁₂ N ₂ O 6	245.078	4.7	194.93	230.1395,178.0735,148.1 123	uridine or its isomer	6	Others	DRTQHJPMGB UCF- XVFCMESISA-N RBJDJJGMGHKQ MI-
28	2.23	C ₃₀ H ₃₈ O ₄	463.2854	2.3	212.74	462.2819,309.1825,230.1 400,145.1013	biatractylenolide/biepiasterolide or isomer	3	Sesquiterpeno id	CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N
29	2.44	C ₁₅ H ₂₀ O ₂	233.1541	2.2	154.56	159.0816,147.0809,141.0 706,128.0625,115.0548,1 05.0705	isomer of atractylenolide II	4	Sesquiterpeno id	-

30	2.65	C ₂₃ H ₂₆ O ₆	399.1814	2.9	158.36	196.1121,159.0928,146.0617	12-seneciolyloxytetradeca-trien-4,6-diyne-1,14-diacetate or its isomer	6	Polyacetylene	BVSZAUUZUUR PHD- AUVZEZIHSA-N RGLXMSBHZCN
31	2.76	C ₂₁ H ₂₀ O ₁₁	449.108	0.4	247.55	365.0704,287.0583,120.0816	luteolin - <i>O</i> -glucoside or its isomer	6	Flavonoid	DGG- AOHSKODXSA- N PZKISQRTNNHU
32	2.83	C ₂₁ H ₂₀ O ₁₁	449.1101	5	246.64	431.0993,395.0769,353.0668,329.0661,299.0557	glucopyranosyloxy-4',5,7-trihydroxy-flavone or its isomer	6	Flavonoid	GF- JDQAKFQDSA-N
33	2.84	C ₁₅ H ₂₀ O	217.1596	4	151.52	200.2017,187.1487,145.1017,128.0624	isomer of atractylon	3	Sesquiterpenoid	-
34	2.86	C ₉ H ₁₂ N ₂ O ₆	245.0778	3.9	199.92	199.1123,188.0721,159.0927,146.0613	uridine or its isomer	6	Others	DRTQHJPMGB UCF- XVFCMESISA-N QQSKRWNYOUT
35	2.88	C ₁₄ H ₁₆ O ₃	233.1186	5.9	146.78	183.0922,141.0702,128.0627	12-hydroxytetradeca-trien-4,6-diyne-1-ol or its isomer	2	Polyacetylene	NSM- FCGWLDPVSA-N
36	2.94	C ₁₆ H ₁₂ O ₅	287.0566	5.5	158.29	255.0850,244.2280,183.0925,162.0412	isomer of luteolin	5	Flavonoid	-
37	2.96	C ₁₅ H ₂₀ O ₂	233.1537	0.4	152.24	186.0926,176.1079,136.0631	isomer of atractylenolide II	5	Sesquiterpenoid	-
38	2.97	C ₁₅ H ₂₀ O	217.1595	4	152.86	193.0738,178.0769,167.0719,160.0768,151.0559,140.0499,120.0816	isomer of atractylon	2	Sesquiterpenoid	-

39	2.98	C ₂₁ H ₃₆ O ₉	433.2448	3.7	232.65	327.1709,265.1804,231.1 135,214.0869	dictamnocide A or its isomer	4	Others	HYCSHXRCGZLJ NW- FPOJDZHTSA-N PZKISQRTNNHU
40	3.03	C ₂₁ H ₂₀ O ₁₁	449.1084	1.3	247.05	431.0969,413.0870,377.0 661,353.0661,299.0555,2 87.0549,120.0812	glucopyranosyloxy-4',5,7- trihydroxy-flavone or its isomer	6	Flavonoid	GF- JDQAKFQDSA-N
41	3.04	C ₁₅ H ₂₀ O	217.1593	2.7	149.55	200.1521,175.1488,141.0 705,128.0624	isomer of atractylon	3	Sesquiterpeno id	-
42	3.1	C ₂₀ H ₃₄ O ₁₀	435.224	3.5	193.31	347.1255,311.1030,265.0 966,211.0873	atractyloside A or isomer	4	Others	TTWARFJENFIGJ K-DNGRJINJSA- N FKPHXQBXXXYI
43	3.17	C ₁₅ H ₂₂ O	219.1752	3.8	150.87	219.1752,162.0781,135.0 669	atractylmacrols D or its isomer	5	Sesquiterpeno id	ON- LTNMDHOVSA- N FBMORZZOJSDN RQ- GLQYFDAESA- N/FBMORZZOJS
44	3.18	C ₁₅ H ₂₀ O ₃	249.149	1.9	155.72	230.0816,203.0838,141.0 700,128.0627	atractylenolide III/ketone- atractylenolide III/epiatractylen olide III or isomer	2	Sesquiterpeno id	DNRQ- GLQYFDAESA- N/ FBMORZZOJSDN RQ- GLQYFDAESA-N

45	3.23	C ₁₅ H ₂₀ O	217.1591	1.7	150.36	193.0350,175.0243,139.0031	isomer of atractylon	4	Sesquiterpenoid	–
46	3.33	C ₁₅ H ₁₈ O ₂	231.1387	3.2	153.43	213.1275,175.1124,165.0708,143.0766,130.0658	isomer of atractylenolide I	2	Sesquiterpenoid	–
47	3.38	C ₂₀ H ₃₄ O ₁₀	435.2239	3.2	198.13	389.2537,352.1608,322.1923,227.1194,175.1159	atractyloside A or isomer	3	Others	TTWARFJENFIGJ K-DNGRJINJSA-N FKPHXQBXXXI
48	3.39	C ₁₅ H ₂₂ O	219.1743	-0.2	151.35	187.1107,163.0396,149.0227,115.0549	atractylmacrols D or its isomer	3	Sesquiterpenoid	ON- LTNMDHOVSA-N QQSKRWNYOUT
49	3.43	C ₁₄ H ₁₆ O ₃	233.1167	-2.1	148.92	187.0770,170.0750,141.0704,128.0623,115.0548	12-hydroxytetradeca-trien-4,6-diy-1-ol or its isomer	2	Polyacetylene	NSM- FCGWLDPVSA-N FBMORZZOJSDN RQ-
50	3.45	C ₁₅ H ₂₀ O ₃	249.1489	1.5	157.35	231.1383,215.1034,197.1491,165.0192,153.0688	atractylenolide III/ketone-atractylenolide III/epiatractylenolide or isomer	3	Sesquiterpenoid	GLQYFDAESA-N/ FBMORZZOJS DNRQ- GLQYFDAESA-N/
51	3.46	C ₁₅ H ₂₀ O ₂	233.1541	2	153.26	187.0771,159.0812,144.0576,131.0863,91.0545	isomer of atractylenolide II	2	Sesquiterpenoid	–

52	3.51	C ₁₅ H ₂₂ O	219.1749	2.7	151.51	186.0924,145.1022,119.0 865,105.0702,91.0545	atractylmacrols D or its isomer	2	Sesquiterpeno id	FKPHXQBXXXI ON- LTNMDHOVSA- N
53	3.56	C ₁₆ H ₁₂ O ₅	287.0556	2	237.18	275.0826,265.0952,249.1 025,219.0916	isomer of luteolin	4	Flavonoid	-
54	3.59	C ₉ H ₆ O ₃	163.0399	5.5	122.47	163.0398,141.0705,128.0 626,115.0548,107.0494	7-hydroxycoumarin or its isomer	1	Coumarin	ORHBXUUXSCN DEV- UHFFFAOYSA-N AODJPEDJOAFD MW- QZKOUSHUSA- N/ ZNJXPXRKVUPZ BL- RZFFKMDDSA-N VDDALGSXMJY
55	3.59	C ₁₅ H ₂₀ O ₄	265.1441	2.4	160.47	159.0931,138.1285,107.0 494	tractylenolide V/epoxy-8 - hydroxyatractylenolide II or isomer	1	Sesquiterpeno id	SIM- MDWZMJQESA- N FKPHXQBXXXI ON- LTNMDHOVSA- N
56	3.61	C ₁₇ H ₂₂ O ₂	259.1702	3.5	163.19	195.0929,152.0626,137.0 606	2-dimethyl-octadienyl-methyl- cyclohexadiene-1,4-dione or its isomer	2	Benzoquinone	
57	3.64	C ₁₅ H ₂₂ O	219.1745	0.8	151.6	165.0706,141.0709,115.0 549	atractylmacrols D or its isomer	2	Sesquiterpeno id	

58	3.68	C ₁₉ H ₂₂ O ₄	315.1598	2.3	172.53	271.0959,195.0798,184.1 130,165.0705,153.0698,1 29.0700	12-seneciolyxotetradeca-trien- 4,6-diyne-1-ol or its isomer	2	Polyacetylene	UJHAKGDWVZI MIT- ADDDGJNWSA- N
59	3.73	C ₂₁ H ₂₄ O ₅	357.1714	5	183.81	314.1131,294.0868,250.1 067,195.0798	14-acetoxy-12- seneciolyxotetradeca-trien-4,6- diyne-1-ol or its isomer	2	Polyacetylene	CQDVFBMTEZF KKY- JPSRSCNUSA-N
60	3.76	C ₂₁ H ₂₆ O ₅	359.1862	2.5	188.13	255.0653,210.1280, 186.1135,167.0709	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyne-1-ol or its isomer	2	Polyacetylene	WJQQGLCBGRP HBP- AUVZEZIHSA-N
61	3.82	C ₁₅ H ₂₀ O	217.1592	2.4	152.05	193.0745,183.0930,169.0 766, 157.1016,129.0700	isomer of atractylon	2	Sesquiterpeno id	-
62	3.87	C ₁₉ H ₂₄ O ₃	301.1789	-3.1	177.55	279.0656,271.0989, 213.0543,158.0606	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol or its isomer	2	Polyacetylene	CNBBGYNWCSL FQW- JHTNEVNSSA-N
63	3.88	C ₁₆ H ₁₂ O ₅	287.0553	1	210.73	269.1907,229.1593,169.1 009, 153.0959	isomer of luteolin	2	Flavonoid	-
64	3.88	C ₂₁ H ₂₀ O ₁₁	449.1078	-0.2	210.56	287.0555,269.1907,153.0 701	luteolin -O-glucoside or its isomer	2	Flavonoid	RGLXMSBHZCN DGG- AOHASKODXSA- N
65	3.91	C ₂₀ H ₂₄ O ₅	345.1695	-0.3	207.92	287.0555,269.1906,255.1 384,198.1132,169.1009,1 58.0959	14-acetoxy-12- methylpropionyltetradeca-trien- 4,6-diyne-1-ol or its isomer	2	Polyacetylene	RLOXIGRNKNT VJQ- JPSRSCNUSA-N

66	3.95	C ₁₀ H ₁₀ O ₄	195.0658	3.1	144.27	173.1082,167.0720,165.0705,159.0924	ferulic acid/ methyl caffeate	1	Others	KSEBMYQBYZT DHS- HWKANZROSA- N/ OCNYGKNIVPVP PX- HWKANZROSA- N
67	3.96	C ₁₀ H ₉ O ₄	193.0501	3	131.55	181.0665,173.1082,157.0664,152.0627,149.0606	isomer of scopoletin	1	Coumarin	-
68	3.99	C ₁₅ H ₂₂	203.1803	4.1	148.16	188.0720,173.1295,167.0828	atractylenolide VI or its isomer	4	Sesquiterpenoid	LSKFMNJTZCRQ EF- CABCVRRESA-N HYCSHXRCGZLJ
69	3.99	C ₂₁ H ₃₆ O ₉	433.2447	3.5	217.89	433.2447,301.0710288.1979, 241.1268	dictamnocide A or its isomer	3	Others	NW- FPOJDZHTSA-N ORHBXUUXSCN
70	4.06	C ₉ H ₆ O ₃	163.0397	4.2	122.44	163.0397,117.0341,89.0389	7-hydroxycoumarin or its isomer	2	Coumarin	DEV- UHFFFAOYSA-N
71	4.15	C ₁₅ H ₂₀ O	217.1595	3.9	148.64	198.1111,180.1017,162.1033	isomer of atractylon	6	Sesquiterpenoid	-
72	4.21	C ₁₅ H ₂₀ O ₂	233.1542	2.7	154.37	215.1433,187.1490,159.1178, 145.1017,105.0704,91.0549	isomer of atractylenolide II	2	Sesquiterpenoid	-

73	4.42	C ₁₅ H ₂₀ O	217.1592	2.4	147.32	217.1592,162.1032,110.0 717	isomer of atractylon	5	Sesquiterpeno id	-
74	4.44	C ₁₀ H ₉ O ₄	193.0502	3.2	128.81	178.0268,161.0244,150.0 319,137.0605	scopoletin	1	Coumarin	RODXRVNMMD RFIK- UHFFFAOYSA-N
75	4.49	C ₉ H ₆ O ₃	163.0396	4.2	122.31	133.0291,122.0367,105.0 341,94.0418,77.0390	7-hydroxycoumarin or its isomer	2	Coumarin	ORHBXUUXSCN DEV- UHFFFAOYSA-N
76	4.51	C ₁₀ H ₁₀ O ₃	179.0702	-0.2	135.55	163.0396,117.0343,89.03 90	methoxycinnamic acid	1	Others	AFDXODALSZR GIH- QPJXXVBHSA-N FKPHXQBXXXYI
77	4.53	C ₁₅ H ₂₂ O	219.1749	2.7	151.37	179.0353,162.0321,133.0 288	atractylmacrols D or its isomer	1	Sesquiterpeno id	ON- LTNMDHOVSA- N AODJPEDJOAFD MW- QZKOUSHUSA- N/ ZNJXPXRKVUPZ BL- RZFFKMDDSA-N
78	4.53	C ₁₅ H ₂₀ O ₄	265.1437	1.1	161.07	145.1019,131.0858,128.0 623,103.0550,91.0545	tractylenolide V/epoxy-8 - hydroxyatractylenolide II or isomer	1	Sesquiterpeno id	

79	4.65	C ₁₅ H ₂₂ O	219.1747	1.8	153.56	201.1642,184.0965,167.0 709,152.0625,129.0699	atractylmacrols D or its isomer	2	Sesquiterpeno id	FKPHXQBXXXVI ON- LTNMDHOVSA- N
80	4.67	C ₁₅ H ₂₀ O ₃	249.1491	2.5	158.93	249.1491,203.1059,174.0 917,162.0322,129.0702 215.1086,187.0757,165.1	isomer of 13-13-hydroxyl- atractylenolide II	1	Sesquiterpeno id	-
81	4.87	C ₁₄ H ₁₆ O ₃	233.1178	2.3	150.09	016,152.0628,128.0626,1 15.0546,105.0703,91.054 4	12-hydroxytetradeca-trien-4,6- diyn-1-ol or its isomer	1	Polyacetylene	QQSKRWNYOUT NSM- FCGWLDPVSA-N
82	5.27	C ₂₁ H ₂₀ O ₁₁	449.1447	0.5	216.89	284.2952,269.1907,243.1 748,181.0500,165.0703,1 28.0624,115.0546	hydroxy-methoxyflavonone-O- glucoside or its isomer	1	Flavonoid	LRIHEGZGXAQ QE- SPQBBPEMSA-N AODJPEDJOAFD
83	5.31	C ₁₅ H ₂₀ O ₄	265.1435	0.3	160.64	233.0806,208.0527,152.0 626,144.0578	tractylenolide V/epoxy-8 - hydroxyatractylenolide II or isomer	1	Sesquiterpeno id	MW- QZKOUSHUSA- N/ FBMORZZOJSDN RQ-
84	5.36	C ₁₅ H ₂₀ O ₃	249.1489	1.6	158.17	185.1330,161.0606,157.1 015,141.0704,129.0697,1 05.0699	atractylenolide III/ketone- atractylenolide III/epiatractylen olide or isomer	1	Sesquiterpeno id	GLQYFDAESA- N/FBMORZZOJS DNRQ- GLQYFDAESA- N/

85	5.37	C ₉ H ₆ O ₃	163.0396	3.6	243.85	145.0293,135.0446,117.0 339, 89.0389	7-hydroxycoumarin or its isomer	2	Coumarin	ORHBXUUXSCN DEV- UHFFFAOYSA-N FKPHXQBXXXYI
86	5.44	C ₁₅ H ₂₂ O	219.1748	2	152.13	159.1166,142.0776,119.0 862,91.0549	atractylmacrols D or its isomer	1	Sesquiterpeno id	ON- LTNMDHOVSA- N QQSKRWNYOUT
87	5.46	C ₁₄ H ₁₆ O ₃	233.1183	4.7	150.55	145.0657,142.0776,119.0 862,91.0548	12-hydroxytetradeca-trien-4,6- diyn-1-ol or its isomer	1	Polyacetylene	NSM- FCGWLDPVSA-N
88 ^a	5.56	C ₁₆ H ₁₂ O ₅	287.0556	2	161.16	287.0558,269.1908,241.0 494, 178.0786,153.0194,137.0 608,121.1018,91.0544	luteolin	1	Flavonoid	IQPNAANSBPBG FQ- UHFFFAOYSA-N
89	5.57	C ₁₅ H ₂₂	203.18	2.7	148.71	181.0497,178.0785,167.0 715,152.0623	atractylenolide VI or its isomer	2	Sesquiterpeno id	LSKFMNJTZRQ EF- CABCVRRESA-N
90	6.01	C ₁₅ H ₂₀ O ₃	249.1493	2.9	156.99	231.1382,185.1332,165.0 705,157.1020,143.0855,1 29.0696,105.0705	isomer of 13-hydroxyl- atractylenolide II	1	Sesquiterpeno id	-
91	6.06	C ₁₅ H ₂₂ O	219.1751	3.3	153.05	189.1267, 155.0862, 142.0774, 133.1019, 105.0705, 91.0546	atractylmacrols D or its isomer	1	Sesquiterpeno id	FKPHXQBXXXYI ON- LTNMDHOVSA- N

92	6.14	C ₁₄ H ₁₆ O ₃	233.1181	3.6	151.56	157.1019,117.0710,77.0388	12-hydroxytetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	QQSKRWNYOUT NSM- FCGWLDPVSA-N
93	6.15	C ₁₅ H ₂₂	203.1798	2.1	149.16	159.1177,133.1019,117.0710,77.0389	atractylenolide VI or its isomer	1	Sesquiterpenoid	LSKFMNJTZCRQ EF- CABCVRRESA-N AHQSJTKTHCKP
94	6.19	C ₁₅ H ₂₄ O	221.1882	-1.7	152.88	157.1020,133.1019,127.0549,117.0710,105.0704,77.0389	atractylmacrols E	1	Sesquiterpenoid	MM- LTNMDHOVSA-N N ORHBXUUXSCN
95	6.25	C ₉ H ₆ O ₃	163.0397	4.6	244.38	145.0291,135.0446,117.0341, 89.0388	7-hydroxycoumarin or its isomer	3	Coumarin	DEV- UHFFFAOYSA-N
96	6.28	C ₁₄ H ₁₆ O ₃	233.1187	6.5	152.86	165.0703,159.0803,128.0623,105.0704	12-hydroxytetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	QQSKRWNYOUT NSM- FCGWLDPVSA-N
97 ^a	6.29	C ₁₅ H ₁₀ O ₅	271.061	3.3	156.55	271.0596,243.1752,165.0703,153.0701,105.0704,91.0546	apigenin	1	Flavonoid	KZNIFHPLKGYR TM- UHFFFAOYSA-N
98	6.29	C ₁₆ H ₁₈ O ₄	275.1287	3.2	164.84	205.0763,180.0815,152.0624,129.0701,91.0546	14-acetoxytetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	OSOQCOKGODM ZLC- HJHGKILDSA-N
99	6.38	C ₂₃ H ₂₆ O ₆	399.1821	4.6	205.59	267.1135,159.0809,156.0930,155.0859,105.0705,	12-seneciolyxytetradeca-trien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	BVSZAUUZUUR PHD- AUVZEZIHSA-N

100	6.44	C ₁₇ H ₂₂ O ₅	307.1545	1.7	174.6	224.1036,198.0755,171.0814	atractylenolide IV or its isomer	1	Sesquiterpenoid	GYTSMBNRXNO QKU- GUDXXQAFSA- N
101	6.76	C ₁₄ H ₁₆ O ₃	233.1182	4.1	148.23	201.1281,178.0783,165.0705,153.0699,128.0623,15.0548,105.0703,77.0388	12-hydroxytetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	QQSKRWNYOUT NSM- FCGWLDPVSA-N
102	6.79	C ₁₉ H ₂₂ O ₄	315.1604	4.2	177.79	201.1281,185.1331,165.0705,157.1020,105.0703	12-seneciolyoxytetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	UJHAKGDWVZI MIT- ADDDGJNWSA- N
103	6.87	C ₁₅ H ₂₂ O	219.1748	2.3	150.09	159.1174,145.1021,135.0812,130.0772	atractylmacrols D or its isomer	1	Sesquiterpenoid	FKPHXQBXXXYI ON- LTNMDHOVSA- N
104	6.94	C ₁₅ H ₂₀ O	217.1592	2.5	153.04	199.1487,175.1125,128.0625, 105.0704	isomer of atractylon	3	Sesquiterpenoid	-
105 ^a	6.96	C ₁₅ H ₂₀ O ₃	249.1492	2.8	157.66	231.1379,213.1285,204.0810,185.1338,161.0252,157.1017,141.0706,105.0547	atractylenolide III	1	Sesquiterpenoid	FBMORZZOJSDN RQ- GLQYFDAESA-N
106	6.96	C ₃₄ H ₄₂ O ₈	579.2932	-3.6	243.93	561.2823,337.2747,313.2747,155.0112	biatractylenolide II or its isomer	6	Sesquiterpenoid	DJINKBUXGFQI CR- GJDTUZTCSA-N

107	7	C ₁₄ H ₁₆ O ₃	233.1178	2.6	150.4	185.1338,155.0859,141.0 705,128.0625,115.0547,9 1.0545	12-hydroxytetradeca-trien-4,6- diyn-1-ol or its isomer	1	Polyacetylene	QQSKRWNYOUT NSM- FCGWLDPVSA-N
108	7.12	C ₂₁ H ₂₆ O ₅	359.1867	3.8	194.36	243.1387,179.0341,164.0 842,149.0608,131.0502,1 03.0547	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyn-1-ol or its isomer	1	Polyacetylene	WJQQGLCBGRP HBP- AUVZEIHSAN
109	7.19	C ₁₅ H ₂₀ O ₂	233.1539	1.3	155.34	185.1336,179.0852,145.1 016,131.0858,117.0707,1 05.0705,91.0546,79.0542	isomer of atractylenolide II	1	Sesquiterpeno id	-
110	7.19	C ₂₃ H ₂₈ O ₆	401.197	2.9	209.25	401.1970,213.0921,185.1 336	12-methylbutyryltetradeca- trien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	YVBOVXWVUL MJDC- NLCRFJRRSA-N
111	7.21	C ₁₅ H ₂₂	203.1801	3.5	148.89	178.0785,165.0704,145.1 016,142.0779,119.0863,1 05.0705	atractylenolide VI or its isomer	1	Sesquiterpeno id	LSKFMNJTZCRQ EF- CABCVRRESA-N
112	7.32	C ₃₄ H ₄₂ O ₈	579.2926	-4.6	244.49	579.2926,534.3191,337.2 740	biatractylenolide II or its isomer	3	Sesquiterpeno id	DJINKBUXGFQI CR- GJDTUZTCSA-N
113	7.42	C ₂₁ H ₂₄ O ₅	357.1702	1.6	183.66	251.1069,237.0921,203.0 707,197.0972,195.0811,1 42.0776	14-acetoxy-12- senecioyloxytetradeca-trien-4,6- diyn-1-ol or its isomer	1	Polyacetylene	CQDVFBMTEZF KKY- JPSRSCNUSA-N
114	7.49	C ₉ H ₆ O ₃	163.0397	4.3	122.37	145.0291,135.0448,117.0 339, 89.0387	7-hydroxycoumarin or its isomer	2	Coumarin	ORHBXUUXSCN DEV- UHFFFAOYSA-N

115	7.55	C ₂₃ H ₂₆ O ₆	399.1809	1.8	208.25	327.1603,267.1380,165.0 705,141.0704	12-seneciolyxytetradeca-trien- 4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	BVSZAUUZUUR PHD- AUVZEZIHSA-N
116	7.61	C ₁₅ H ₂₀ O ₃	249.1491	2.2	155.61	213.1283,203.1447,185.1 333,143.0855,105.0703	isomer of 13-hydroxyl- atractylenolide II	1	Sesquiterpeno id	-
117	7.63	C ₁₅ H ₁₈ O ₂	231.1385	2.4	152.94	213.1283,185.1334,157.1 016,143.0855,128.0624,1 15.0548	isomer of atractylenolide I	1	Sesquiterpeno id	-
118	7.85	C ₁₉ H ₂₂ O ₄	315.1602	3.6	178.01	269.1546,185.1331,141.0 706,128.0624,	12-seneciolyxytetradeca-trien- 4,6-diyne-1-ol or its isomer	1	Polyacetylene	UJHAKGDWVZI MIT- ADDDGJNWSA- N
119	7.92	C ₂₁ H ₂₆ O ₅	359.1858	1.4	192.22	341.1764,269.1549,243.1 384,119.0862	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyne-1-ol or its isomer	1	Polyacetylene	WJQQGLCBGRP HBP- AUVZEZIHSA-N FKPHXQBXXXI
120	7.94	C ₁₅ H ₂₂ O	219.1747	1.7	151.25	187.1119,154.0765,141.0 703	atractylmacrols D or its isomer	1	Sesquiterpeno id	ON- LTNMDHOVSA- N
121	7.99	C ₉ H ₆ O ₃	163.0397	4.4	228.54	163.0397,145.0290,135.0 449, 117.0342	7-hydroxycoumarin or its isomer	2	Coumarin	ORHBXUUXSCN DEV- UHFFFAOYSA-N
122	7.99	C ₂₀ H ₂₄ O ₅	345.1723	7.7	186.62	324.1974,282.1490,271.1 701,165.0704	14-acetoxy-12- methylpropionyltetradeca-trien- 4,6-diyne-1-ol or its isomer	1	Polyacetylene	RLOXIGRNKNT VJQ- JPSRSCNUSA-N

123	8	C ₁₉ H ₂₄ O ₄	317.175	0.9	179.25	204.0843,179.0844,165.0704	14-methylbutyryltetradecatrien-4,6-diyn-1-ol or its isomer	1	Polyacetylene	ILXATFYUJVFIQ N- ADDDGJNWSA- N XDSKMYLDYJ
124	8.23	C ₁₉ H ₂₂ O ₃	299.1666	8.2	173.15	187.1125,169.1018,159.0818,131.0503	14-seneciolyxytetradecatrien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	PBI- JHTNEVNSSA-N
125	8.25	C ₁₅ H ₂₀ O	217.1594	3	148.12	183.1184,170.1096,157.1017,155.0860,153.0701,142.0776,128.0626,119.0863	isomer of atractylon	1	Sesquiterpenoid	-
126	8.25	C ₁₇ H ₂₂ O ₅	307.1548	2.5	176.29	241.1459,187.1126,175.0760,119.0863,105.0704,103.0549	atractylenolide IV or its isomer	1	Sesquiterpenoid	GYTSMBNRXNO QKU- GUDXXQAFSA- N
127	8.34	C ₂₁ H ₂₆ O ₅	359.1861	2.2	190.48	328.1678,298.0890,267.1388,231.1385,181.1019	14-acetoxy-12-methylbutyryltetradecatrien-4,6-diyn-1-ol	1	Polyacetylene	GZYILNTUJVFIQ HX- JPSRSCNUSA-N
128	8.35	C ₁₆ H ₁₈ O ₄	275.1297	7.1	168.45	178.0788,158.0956,116.0595	14-acetoxytetradecatrien-4,6-diyn-1-ol or its isomer	1	Polyacetylene	OSOQCOKGODM ZLC- HJHGIKLDSA-N
129	8.4	C ₁₇ H ₂₂ O ₅	307.1549	2.9	175.64	246.1520,230.1387,188.101,187.1122,173.0968,159.0812,145.0651,131.0861	atractylenolide IV or its isomer	1	Sesquiterpenoid	GYTSMBNRXNO QKU- GUDXXQAFSA- N

130	8.55	C ₂₃ H ₂₈ O ₆	401.1984	6.3	203.35	324.2904,119.0861,117.0 707,91.0548	12-methylbutyryltetradeca- trien-4,6-diyne-1,14-diacetate or its isomer	2	Polyacetylene	YVBOVXWVUL MJDC- NLCRFJRRSA-N
131	8.58	C ₁₅ H ₁₈ O ₂	231.1387	3.1	152.97	213.1282,185.1330,155.0 861,141.0705,128.0624,1 15.0547,105.0703,91.054 7	isomer of atractylenolide I	1	Sesquiterpeno id	-
132	8.65	C ₂₁ H ₂₆ O ₅	359.1856	1	192.69	324.1947,204.0797,178.0 783,152.0624	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyne-1-ol or its isomer	1	Polyacetylene	WJQQGLCBGRP HBP- AUVZEIHSAN AHGDPGLNCMV
133	8.72	C ₁₈ H ₂₈ O ₃	293.2116	1.5	180.32	293.2116,243.1395,183.1 176	atractylmacrols C or its isomer	1	Sesquiterpeno id	GMO- LXOFESCASAN BVSZAUUZUUR
134	8.78	C ₂₃ H ₂₆ O ₆	399.1814	3	205.75	350.2109,223.1116,183.1 177,181.1036,165.0704	12-seneciolyloxytetradeca-trien- 4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	PHD- AUVZEIHSAN ORHBXUUXSCN
135	8.79	C ₉ H ₆ O ₃	163.0396	3.7	285.42	145.0290,135.0450,117.0 343, 89.0388	7-hydroxycoumarin or its isomer	2	Coumarin	DEV- UHFFFAOYSA-N
136	8.8	C ₂₁ H ₂₆ O ₅	359.186	2	191.86	341.1758,265.1231,255.1 385,199.1121,179.0855,1 67.0867,128.0624,91.054 6	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyne-1-ol or its isomer	1	Polyacetylene	WJQQGLCBGRP HBP- AUVZEIHSAN

137	8.81	C ₁₉ H ₂₄ O ₄	317.1739	-2.7	180.38	270.1599,185.0973,165.0704,155.0861,128.0624	14-methylbutyryltetradecatrien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	ILXATFYUJVFIQ N- ADDDGJNWSA- N
138	8.87	C ₁₅ H ₂₂	203.1801	3.5	147.89	175.0162,165.0705,141.0707,119.0861	atractylenolide VI or its isomer	1	Sesquiterpenoid	LSKFMNJTZCRQ EF- CABCVRRESA-N BVSZAUUZUUR
139	8.9	C ₂₃ H ₂₆ O ₆	399.1821	4.8	208.42	259.1696,215.1437,185.1336,119.0860	12-seneciolyxytetradecatrien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	PHD- AUVZEZIHSA-N YVBOVXWVUL
140	8.95	C ₂₃ H ₂₈ O ₆	401.1964	1.3	197.6	269.1550,242.1555,185.1336,117.0705	12-methylbutyryltetradecatrien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	MJDC- NLCRFJRRSA-N
141	8.98	C ₁₅ H ₂₀ O ₂	233.1543	2.9	152.35	215.1080,187.0768,159.1177,145.1023,131.0862,117.0707,105.0705	isomer of atractylenolide II	1	Sesquiterpenoid	–
142	9.05	C ₁₉ H ₂₂ O ₄	315.1589	-0.6	179.66	283.1710,167.0870,153.0700,128.0624,115.0547	12-seneciolyxytetradecatrien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	UJHAKGDWVZI MIT- ADDDGJNWSA- N
143	9.18	C ₃₄ H ₄₂ O ₈	579.2928	-4.2	244.86	433.1543,377.0920,331.1312,227.0473	biatractylenolide II or its isomer	3	Sesquiterpenoid	DJINKBUXGFQI CR- GJDTUZTCSA-N
144	9.21	C ₁₅ H ₂₀ O ₂	233.1542	2.6	153.41	215.1443,187.1489,165.0709,159.1179	isomer of atractylenolide II	1	Sesquiterpenoid	–

145	9.21	C ₁₇ H ₂₂ O ₂	259.1701	3.2	160.4	259.1701,244.1703,187.1489	2-dimethyl-octadienyl-methyl-cyclohexadiene-1,4-dione or its isomer	1	Benzoquinone	VDDALGSXMJY SIM- MDWZMJQESA- N
146	9.28	C ₂₁ H ₃₆ O ₉	433.2413	-4.5	277.91	433.2413,415.2122,119.0860	dictamnocide A or its isomer	5	Others	HYCSHXRCGZLJ NW- FPOJDZHTSA-N
147	9.31	C ₂₁ H ₂₄ O ₅	357.171	3.8	192.37	341.1765,299.1650,269.1542,253.1227,183.0810	14-acetoxy-12-seneciolyxytetradeca-trien-4,6-diyn-1-ol or its isomer	1	Polyacetylene	CQDVFBMTEZF KKY- JPSRSCNUSA-N
148	9.36	C ₁₅ H ₂₀ O	217.1596	4.2	149.32	199.1123,183.1182,171.0819,155.0860,152.0625,128.0624	isomer of atractylon	1	Sesquiterpenoid	-
149	9.5	C ₂₁ H ₂₆ O ₅	359.1867	4	195.31	287.1656,243.1393,199.1486,1778.0782,155.0859,128.0626,115.0548,104.0626,91.0545	14-acetoxy-12-methylbutyryltetradeca-trien-4,6-diyn-1-ol or its isomer	1	Polyacetylene	WJQQGLCBGRP HBP- AUVZEZHSA-N
150	9.54	C ₁₅ H ₂₀ O	217.1594	3.2	149.26	199.1487,183.0828,171.184,157.1018,143.0863,141.0706,133.0653,128.0626	isomer of atractylon	1	Sesquiterpenoid	-
151	9.63	C ₂₁ H ₂₄ O ₅	357.1708	3.1	193.14	338.2125,293.1561,263.1452,213.1280,149.0603	14-acetoxy-12-seneciolyxytetradeca-trien-4,6-diyn-1-ol or its isomer	1	Polyacetylene	CQDVFBMTEZF KKY- JPSRSCNUSA-N

152	9.76	C ₂₃ H ₂₆ O ₆	399.1813	2.6	206.82	229.1230,195.0816,175.0 759,141.0704,119.0860,1 17.0704,91.0546	12-seneciolyxytetradeca-trien- 4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	BVSZAUUZUUR PHD- AUVZEIHSAN
153	9.78	C ₁₅ H ₂₀ O	217.1594	3.4	148.97	199.1491,183.1172,171.0 820,157.0654,152.0626,1 43.0859,129.0700	isomer of atractylon	1	Sesquiterpeno id	-
154	9.93	C ₁₅ H ₁₈ O ₂	231.1386	2.9	152.44	185.1330,157.1020,128.0 623,105.0703,91.0546	isomer of atractylenolide I	1	Sesquiterpeno id	-
155	9.97	C ₂₃ H ₂₆ O ₆	399.1603	1.2	208.09	339.1603,327.1588,265.1 236,179.0854,165.0703,1 29.0700,91.0545	12-seneciolyxytetradeca-trien- 4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	BVSZAUUZUUR PHD- AUVZEIHSAN
156	10.03	C ₁₅ H ₂₀ O ₂	233.154	1.6	152.52	233.1538,215.1435,187.0 770,185.0968,145.1021,1 31.0859	isomer of atractylenolide II	1	Sesquiterpeno id	-
157	10.04	C ₁₉ H ₂₂ O ₃	299.165	2.8	174.58	243.1389,185.0968,168.0 949,159.0812,131.0859,7 7.0388 32	14-seneciolyxytetradeca-trien- 4,6-diyne-1-ol or its isomer	1	Polyacetylene	XDSKMYLDYJ PBI- JHTNEVNSSAN UJHAKGDWVZI
158	10.05	C ₁₉ H ₂₂ O ₄	315.1602	3.5	177.8	243.1389,182.0958,137.0 606	12-seneciolyxytetradeca-trien- 4,6-diyne-1-ol or its isomer	1	Polyacetylene	MIT- ADDDGJNWSAN
159	10.11	C ₂₃ H ₂₈ O ₆	401.1971	3.2	207.09	287.1654,227.1078,147.0 813,143.0858,119.0861,1 17.0705,115.0548,105.07 01,103.0547,91.0546	12-methylbutyryltetradeca- trien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	YVBOVXWVUL MJDC- NLCRFJRRSAN

160	10.12	C ₂₁ H ₂₄ O ₅	357.1706	2.6	193.65	339.1601,311.1659,259.1 335,205.1034,	14-acetoxy-12-seneciolyxytetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	CQDVFBMTEZF KKY- JPSRSCNUSA-N ILXATFYUJVFIQ
161	10.14	C ₁₉ H ₂₄ O ₄	317.1766	6	178.61	301.1438,256.2079,244.1 709,157.1015	14-methylbutyryltetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	N- ADDDGJNWSA- N
162	10.24	C ₂₃ H ₂₆ O ₆	399.1818	3.9	208.11	339.1604,267.1344,241.1 240,195.0812,165.0705,1 28.0624,115.0548,91.054 6	12-seneciolyxytetradeca-trien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	BVSZAUUZUUR PHD- AUVZEIHSAN
163	10.35	C ₁₉ H ₂₄ O ₄	317.1749	0.7	176.38	284.2023,274.2174,269.1 545,231.1387,183.0813,1 57.1017,129.0697,117.07 05,91.0546	14-methylbutyryltetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	N- ADDDGJNWSA- N
164	10.36	C ₂₃ H ₂₈ O ₆	401.1961	0.7	204.42	287.1644,185.0977,157.1 016,145.1018,119.0863,1 17.0705,91.0546	12-methylbutyryltetradeca-trien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	YVBOVXWVUL MJDC- NLCRFJRRSAN
165	10.44	C ₁₆ H ₁₈ O ₄	275.1275	-1.1	162.96	243.1385,179.0843,145.1 019	14-acetoxytetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	OSOQCOKGODM ZLC- HJHGKLDSAN
166	10.59	C ₁₅ H ₂₀ O ₃	249.1491	2.2	157.16	230.1550,214.1236,184.1 125,170.0966,141.0704	isomer of 13-hydroxyl-atractylenolide II	1	Sesquiterpenoid	-
167	10.68	C ₁₅ H ₂₀ O ₂	233.1542	2.6	154.13	215.1441,187.1490,159.1 174,145.1018,105.0706,9 1.0546,79.0545	isomer of atractylenolide II	1	Sesquiterpenoid	-

168 ^a	10.95	C ₁₅ H ₂₀ O ₂	233.1544	3.3	154.09	215.1437,187.1493,159.177,105.0701	atractylenolide II	1	Sesquiterpenoid	OQYBLUDOFO BPO- KCQAQPDRSA-N WJQQGLCBGRP
169	11.18	C ₂₁ H ₂₆ O ₅	359.1864	3.1	189.31	280.2640,213.1279,199.122,107.0500	14-acetoxy-12-methylbutyryltetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	HBP- AUVZEZIHSAN UJHAKGDWVZI
170	11.23	C ₁₉ H ₂₂ O ₄	315.1593	0.7	177.29	262.2535,216.1760,165.0705,115.0548,91.0547	12-seneciolyxytetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	MIT- ADDDGJNWSAN
171	11.51	C ₂₃ H ₂₈ O ₆	401.1952	-1.6	196.82	328.1660,255.1395,247.1348,172.0892,166.0755	12-methylbutyryltetradeca-trien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	YVBOVXWVUL MJDC- NLCRFJRRSAN
172	11.54	C ₁₅ H ₂₀ O ₂	233.1541	2	153.26	215.1441,185.0970,179.0847,159.0814	isomer of atractylenolide II	1	Sesquiterpenoid	–
173	11.56	C ₁₈ H ₂₈ O ₃	293.2116	1.5	178.91	253.1600,242.1547,204.0823	atractylmacrols C or its isomer	1	Sesquiterpenoid	AHGDPGLNCMV GMO- LXOFESCASAN
174	11.59	C ₂₀ H ₂₄ O ₅	345.1715	5.3	187.04	327.1612,243.1386,178.0782	14-acetoxy-12-methylpropionyltetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	RLOXIGRNKNT VJQ- JPSRSCNUSAN
175	11.67	C ₁₅ H ₂₀ O	217.1594	3.5	148.85	199.1488,171.1180,157.1020,143.0863,131.0867,119.0861	isomer of atractylon	1	Sesquiterpenoid	–

176	11.8	C ₁₉ H ₂₄ O ₄	317.1759	3.6	182.43	257.1546,243.1391,129.0701	14-methylbutyryltetradecatrien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	ILXATFYUJVFIQ N- ADDDGJNWSA- N FKPHXQBXXXYI
177	11.86	C ₁₅ H ₂₂ O	219.1748	2	150.11	159.1179,143.0858,131.0862,77.0390	atractylmacrols D or its isomer	1	Sesquiterpenoid	ON- LTNMDHOVSA- N
178	11.91	C ₁₅ H ₂₂	203.1801	3.3	148.21	173.1334,145.1017,142.0776,131.0862	atractylenolide VI or its isomer	1	Sesquiterpenoid	LSKFMNJTZCRQ EF- CABCVRRESA-N
179	12.04	C ₂₃ H ₂₈ O ₆	401.1972	3.4	196.09	328.1672,313.1424,301.1432,241.1245,205.0490,167.0865	12-methylbutyryltetradecatrien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	YVBOVXWVUL MJDC- NLCRFJRRSA-N
180	12.11	C ₁₅ H ₂₂	203.1801	3.2	148.62	183.1177,159.1175,143.0858,119.0864,117.0706	atractylenolide VI or its isomer	1	Sesquiterpenoid	LSKFMNJTZCRQ EF- CABCVRRESA-N
181	12.17	C ₁₇ H ₂₂ O ₂	259.1697	1.8	161.04	259.1697,229.1594,217.1019,193.1019	2-dimethyl-octadienyl-methylcyclohexadiene-1,4-dione or its isomer	1	Benzoquinone	VDDALGSXMJY SIM- MDWZMJQESA- N
182	12.19	C ₁₄ H ₁₆ O ₃	233.1181	3.8	147.73	153.0699,152.0625,127.0549,91.0547	12-hydroxytetradecatrien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	QQSKRWNYOUT NSM- FCGWLDPVSA-N
183	12.24	C ₁₅ H ₂₀ O ₂	233.154	1.8	152.86	185.1334,177.0700,152.0627,145.1019,133.1018	isomer of atractylenolide II	1	Sesquiterpenoid	-

184	12.39	C ₁₉ H ₂₄ O ₃	301.1813	4.8	178.04	197.0967,185.1331,171.0 812,143.0861,128.0624,1 15.0546,91.0546	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	CNBBGYNWCSL FQW- JHTNEVNSSA-N AHGDPGLNCMV
185	12.41	C ₁₈ H ₂₈ O ₃	293.2116	1.7	178.46	185.1332,155.0862,143.0 861,121.0657	atractylmacrols C or its isomer	1	Sesquiterpeno id	GMO- LXOFESCASA-N CQDVFMBMTEZF
186	12.42	C ₂₁ H ₂₄ O ₅	357.1709	3.5	192.13	341.1754,269.1542,159.0 809,142.0781,128.0624,1 15.0546,91.0548	14-acetoxy-12- senecioyloxytetradeca-trien-4,6- diyn-1-ol or its isomer	1	Polyacetylene	KKY- JPSRSCNUSA-N LSKFMNJTZCRQ
187	12.65	C ₁₅ H ₂₂	203.1803	4.2	145.86	179.0855,165.0706,145.1 019,142.0778,119.0864,1 05.0703	atractylenolide VI or its isomer	1	Sesquiterpeno id	EF- CABCVRRESA-N
188	12.66	C ₁₅ H ₂₀ O	217.1595	3.9	148.87	199.1125,185.0970,183.1 174,171.0811,157.1021,1 47.1177,145.1019,131.08 63,117.0706,105.0703,79. 0548	isomer of atractylon	1	Sesquiterpeno id	–
189	12.74	C ₂₃ H ₂₈ O ₆	401.1971	2.1	196.29	328.1673,313.1440,267.1 024,205.0502,165.0707,9 1.0546	12-methylbutyryltetradeca- trien-4,6-diyne-1,14-diacetate or its isomer	1	Polyacetylene	YVBOVXWVUL MJDC- NLCRFJRSA-N
190 ^a	12.99	C ₁₅ H ₁₈ O ₂	231.1385	3	152.42	231.1389,213.1278,185.1 329,157.1018,155.0859,1 43.0703,141.0703,128.06 24,115.0547,91.0543,77.0 387,65.0388	atractylenolide I	1	Sesquiterpeno id	ZTVSGQPHMUY CRS- SWLSCSKDSA-N

191 ^a	13	C ₁₃ H ₁₀ O	183.081	3.07	131.39	183.0806,169.0649,154.0770	atractylodin	1	Sesquiterpenoid	GRBKWAXRYIIT KG- QFMFQGICSA-N AODJPEDJOAFD MW- QZKOUSHUSA- N/ ZNJXPXRKVUPZ BL- RZFFKMDDSA-N RLOXIGRNKNT
192	13.01	C ₁₅ H ₂₀ O ₄	265.1443	3.3	161.22	265.1443,201.0919,155.0859	tractylenolide V/epoxy-8 - hydroxyatractylenolide II or isomer	1	Sesquiterpenoid	VJQ- JPSRSCNUSA-N XDSKMYLDYJ PBI- JHTNEVNSSA-N
193	13.11	C ₂₀ H ₂₄ O ₅	345.1682	-4.3	186.65	317.1335,303.1174,237.0921165.0703,115.0547	14-acetoxy-12- methylpropionyltetradeca-trien- 4,6-diyn-1-ol or its isomer	1	Polyacetylene	FQW- JHTNEVNSSA-N
194	13.12	C ₁₉ H ₂₂ O ₃	299.1659	5.7	174.8	255.1182,234.1294,219.168,206.0975	14-seneciolyloxytetradeca-trien- 4,6-diyn-1-ol or its isomer	1	Polyacetylene	–
195	13.57	C ₁₉ H ₂₄ O ₃	301.1807	2.8	177.65	200.1190,187.1122,171.0811,165.0703,153.0694,143.0856,128.0625,115.0547,91.0545	14-methylbutyryltetradeca- trien-4,6-diyn-1-ol or its isomer	1	Polyacetylene	WJQQGLCBGRP HBP- AUVZEIHSAN
196	13.65	C ₁₅ H ₁₈ O ₂	231.1384	2	152.51	231.1145,184.0739,159.180,143.0858,128.0626	isomer of atractylenolide I	1	Sesquiterpenoid	–
197	13.7	C ₂₁ H ₂₆ O ₅	359.1863	2.7	197.61	289.1024,285.1874,269.1542	14-acetoxy-12- methylbutyryltetradeca-trien- 4,6-diyn-1-ol or its isomer	1	Polyacetylene	–

198	13.77	C ₁₅ H ₂₀ O ₃	249.1491	2.3	235.29	231.1385,203.1441,185.1 331,161.0603,129.0698,1 05.0702,91.0553,79.0559	isomer of 13-hydroxyl- atractylenolide II	1	Sesquiterpeno id	-
199	13.84	C ₁₉ H ₂₄ O ₃	301.1807	3	180.17	269.1549,253.1236,197.0 971,181.1023,169.1019,1 55.0860,128.0626,115.05 47,105.0703,91.0546	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	CNBBGYNWCSL FW- JHTNEVNSSA-N
200	14.16	C ₁₇ H ₂₂ O ₂	259.1698	2.1	163.48	179.0857,165.0701,153.0 696,128.0624	2-dimethyl-octadienyl-methyl- cyclohexadiene-1,4-dione or its isomer	1	Benzoquinone	VDDALGSXMJY SIM- MDWZMJQESA- N FKPHXQBXXXI
201	14.19	C ₁₅ H ₂₂ O	219.1749	2.6	152.91	154.0781,130.0771,105.0 702, 91.0544	atractylmacrols D or its isomer	1	Sesquiterpeno id	ON- LTNMDHOVSA- N
202	14.38	C ₁₅ H ₂₀ O ₂	233.1541	2.2	153.84	187.1494,165.0705,157.1 021, 142.0780,105.0704	isomer of atractylenolide II	1	Sesquiterpeno id	-
203	14.92	C ₁₉ H ₂₂ O ₃	299.1649	2.3	175.2	171.0816,165.0704,155.0 861,142.0777,129.0697,1 15.0548,91.0545	14-seneciolyloxytetradeca-trien- 4,6-diyne-1-ol or its isomer	1	Polyacetylene	XDSKMYLDYJ PBI- JHTNEVNSSA-N ILXATFYUJVFIQ
204	15	C ₁₉ H ₂₄ O ₄	317.1762	4.7	180.82	299.1646,283.1704,167.0 863	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	N- ADDDGJNWSA- N

205	15.14	C ₁₉ H ₂₄ O ₃	301.1803	1.5	177.86	255.1746,216.0911,178.0 329,150.0457	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	CNBBGYNWCSL FW- JHTNEVNSSA-N
206	15.4	C ₁₉ H ₂₄ O ₃	301.1805	2.2	177.51	258.1550,217.1595,199.1 125,169.1018,128.0625,1 05.0703	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	CNBBGYNWCSL FW- JHTNEVNSSA-N ILXATFYUJVFIQ
207	15.44	C ₁₉ H ₂₄ O ₄	317.1755	2.3	180.1	301.1834,257.1545,187.1 121,131.0862	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	N- ADDDGJNWSA- N HYCSHXRCGZLJ
208	15.49	C ₂₁ H ₃₆ O ₉	433.2426	-1.4	290.52	415.2327,353.1573,296.1 573,296.1573,181.0866,1 27.0397	dictamnocide A or its isomer	1	Others	NW- FPOJDZHTSA-N
209	15.55	C ₁₅ H ₂₀ O	217.1591	1.9	149.11	171.1175,167.0866,157.1 021,142.0785,129.0695	isomer of atractylon	1	Sesquiterpeno id	- AODJPEDJOAFD MW- QZKOUSHUSA- N/ ZNJXPXRKVUPZ BL- RZFFKMDDSA-N
210	15.57	C ₁₅ H ₂₀ O ₄	265.144	2.3	161.59	217.1597,159.1178,91.05 46	tractylenolide V/epoxy-8 - hydroxyatractylenolide II or isomer	1	Sesquiterpeno id	- AODJPEDJOAFD MW- QZKOUSHUSA- N/ ZNJXPXRKVUPZ BL- RZFFKMDDSA-N
211	15.63	C ₁₀ H ₁₂ O ₄	197.0816	3.7	222.03	197.0815,189.0918,175.0 759,163.0760,154.0783	isomer of hydroxy-1-(4- hydroxy-3- methoxyphenyl) propan-1-one	1	Coumarin	-

212	15.93	C ₁₅ H ₂₂ O	219.1747	1.8	149.58	201.1639,169.1016,159.1 174,119.0861,77.0388	atractylmacrols D or its isomer	1	Sesquiterpeno id	FKPHXQBXXXXYI ON- LTNMDHOVSA- N
213	15.95	C ₃₄ H ₄₂ O ₈	579.2929	-4	243.21	484.3728,367.3214,338.2 780	biatractylenolide II or its isomer	2	Sesquiterpeno id	DJINKBUXGFQI CR- GJDTUZTCSA-N CNBBGYNWCSL
214	16.03	C ₁₉ H ₂₄ O ₃	301.18	0.6	174.39	287.1646,255.0819,239.0 859,191.1070,165.0706,1 59.0811	14-methylbutyryltetradeca- trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	FQW- JHTNEVNSSA-N AODJPEDJOAFD MW- QZKOUSHUSA- N/ ZNXXPXKRVUPZ BL- RZFFKMDDSA-N
215	16.05	C ₁₅ H ₂₀ O ₄	265.1438	1.3	160.23	227.1438,202.0785,175.0 759	tractylenolide V/epoxy-8 - hydroxyatractylenolide II or isomer	1	Sesquiterpeno id	DJINKBUXGFQI CR- GJDTUZTCSA-N VDDALGSXMJY
216	16.25	C ₃₄ H ₄₂ O ₈	579.2974	3.8	247.19	505.2918,493.2985,464.2 578,458.2147,414.2493,	biatractylenolide II or its isomer	1	Sesquiterpeno id	SIM- MDWZMJQESA- N
217	16.38	C ₁₇ H ₂₂ O ₂	259.1699	2.4	163.41	201.1283,163.0763,151.0 762, 137.0610	2-dimethyl-octadienyl-methyl- cyclohexadiene-1,4-dione or its isomer	1	Benzoquinone	

218	16.82	C ₁₀ H ₁₂ O ₄	197.0815	3.6	226.9	197.0815,184.0741,157.1020,127.0397	hydroxy-1-(4-hydroxy-3-methoxyphenyl) propan-1-one	1	Coumarin	NXCPMSUBVRG TSE- UHFFFAOYSA-N
219	17.04	C ₁₇ H ₂₂ O ₂	259.1697	1.8	162.5	175.0761,161.0605,137.0599	2-dimethyl-octadienyl-methyl-cyclohexadiene-1,4-dione or its isomer	1	Benzoquinone	VDDALGSXMJY SIM- MDWZMJQESA-N
220	17.1	C ₁₅ H ₂₀ O	217.1592	2.2	148.85	199.1122,184.0739,142.0778,129.0700,115.0547,105.0704	isomer of atractylon	1	Sesquiterpenoid	-
221	17.29	C ₃₄ H ₄₂ O ₈	579.2927	-4.3	243.79	507.4049,337.2744,313.2745, 277.2170	biatractylenolide II or its isomer	2	Sesquiterpenoid	DJINKBUXGFQI CR- GJDTUZTCSA-N
222	17.39	C ₂₀ H ₂₄ O ₅	345.1674	-6.5	183.94	330.1390,289.1021,242.1559,214.1329,202.0792	14-acetoxy-12-methylpropionyltetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	RLOXIGRNKNT VJQ- JPSRSCNUSA-N AODJPEDJOAFD MW-
223	17.4	C ₁₅ H ₂₀ O ₄	265.1442	2.9	160.27	215.1437,167.0861,155.0862	tractylenolide V/epoxy-8-hydroxyatractylenolide II or isomer	1	Sesquiterpenoid	QZKOUSHUSA-N/ ZNJXPXRKVUPZ BL-
224	17.59	C ₁₈ H ₂₈ O ₃	293.2118	2.4	180.28	230.1581,200.1129,105.0703,79.0544	atractylmacrols C or its isomer	1	Sesquiterpenoid	RZFFKMDDSA-N AHGDPGLNCMV GMO- LXOFESCASA-N

225	17.61	C ₂₉ H ₄₈ O	413.3781	0.8	222.84	413.3781,395.3684,387.3110, 385.2966	stigmaterol	2	Others	HCXVJBMSMIA RIN- SGUOLBJQSA-N
226	17.64	C ₂₀ H ₂₄ O ₅	345.1667	3	185.62	331.1495,289.1020,243.1386,105.0702,79.0544	14-acetoxy-12-methylpropionyltetradeca-trien-4,6-diyne-1-ol or its isomer	1	Polyacetylene	RLOXIGRNKNT VJQ- JPSRSCNUSA-N
227 ^a	18.04	C ₁₅ H ₂₀ O	217.1593	2.6	148.76	199.1124,171.1179,157.1015,141.0704,131.0858,128.0627,119.0864	atractylon	1	Sesquiterpenoid	TYPVSDGIQA AD- HIFRSBDPSA-N RBJDJJGMGHKQ MI-
228	18.3	C ₃₀ H ₃₈ O ₄	463.284	-0.5	226.94	447.2908,433.2754,389.2490,325.1808,233.1555	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpenoid	CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N LSKFMNJTZCRQ
229	18.48	C ₁₅ H ₂₂	203.1799	2.3	147.06	185.1332,159.1175,145.1018,119.0860	atractylenolide VI or its isomer	1	Sesquiterpenoid	EF- CABCVRRESA-N
230	18.52	C ₁₅ H ₁₈ O ₂	231.1385	2.2	152.38	201.0918,185.1332,159.1174,157.1019,143.0859,128.0626,115.0549	isomer of atractylenolide I	1	Sesquiterpenoid	-
231	18.78	C ₁₅ H ₁₈ O ₂	231.1385	2.2	152.09	185.1334,155.0861,128.0627,91.0545	isomer of atractylenolide I	1	Sesquiterpenoid	-

232	18.86	C ₃₀ H ₃₈ O ₄	463.285	1.6	221.76	445.2751,431.2592,427.2 270,394.2108,215.0866,1 84.0740,121.0643,79.054 3	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpeno id	RBJDJJGMGHKQ MI- CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N
233	19	C ₁₅ H ₂₂	203.1803	4.2	146.53	184.0741,173.1330,145.1 019,119.0865,105.0707	atractylenolide VI or its isomer	1	Sesquiterpeno id	LSKFMNJTZCRQ EF- CABCVRRESA-N RBJDJJGMGHKQ MI- CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N
234	19.1	C ₃₀ H ₃₈ O ₄	463.2845	0.5	216.41	447.2920,417.2801,384.2 352,341.1768,231.1389,1 84.0741	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpeno id	DJINKBUXGFQI CR- GJDTUZTCSA-N
235	19.15	C ₃₄ H ₄₂ O ₈	579.2928	-4.3	243.95	579.2928,550.3412,395.3 543	biatractylenolide II or its isomer	2	Sesquiterpeno id	–
236	19.24	C ₁₅ H ₂₀ O ₂	233.1537	0.5	154.55	185.1331,155.0859,129.0 698,115.0550	isomer of atractylenolide II	1	Sesquiterpeno id	VDDALGSXMJY SIM- MDWZMJQESA- N
237	19.77	C ₁₇ H ₂₂ O ₂	259.1699	2.6	169.06	219.1698,163.1123,147.0 811,107.0496	2-dimethyl-octadienyl-methyl-- cyclohexadiene-1,4-dione or its isomer	5	Benzoquinone	

238	19.93	C ₁₅ H ₁₈ O ₂	231.1386	3	152.18	213.1284,201.0918,185.1 332,155.0862,141.0705,1 28.0625,115.0550	isomer of atractylenolide I	1	Sesquiterpeno id	-
239	19.95	C ₃₄ H ₄₂ O ₈	579.2925	-4.7	243.72	550.426,531.2732,337.27 41,263.1287	biatractylenolide II or its isomer	5	Sesquiterpeno id	DJINKBUXGFQI CR- GJDTUZTCSA-N
240	20.43	C ₃₄ H ₄₂ O ₈	579.2925	-4.7	243.93	579.2925,550.3414,337.2 743	biatractylenolide II or its isomer	2	Sesquiterpeno id	DJINKBUXGFQI CR- GJDTUZTCSA-N RBJDJJGMGHKQ MI-
241	20.59	C ₃₀ H ₃₈ O ₄	463.2842	-0.2	222.79	339.1675,199.0753,175.1 134,121.1022	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpeno id	CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N RBJDJJGMGHKQ MI-
242	20.76	C ₃₀ H ₃₈ O ₄	463.285	1.5	220.8	447.2877,313.1883,177.0 916,79.0549	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpeno id	CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N

243	21.41	C ₃₀ H ₃₈ O ₄	463.2848	1.1	228.78	445.2746,417.2790,315.1 976,243.1385,229.1237,1 49.0967,121.1020	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpeno id	RBJDJJGMGHKQ MI- CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N VDDALGSXMJY
244	21.6	C ₁₇ H ₂₂ O ₂	259.1697	1.8	161.2	203.1074,189.0918,175.0 760	2-dimethyl-octadienyl-methyl- cyclohexadiene-1,4-dione or its isomer	1	Benzoquinone	SIM- MDWZMJQESA- N RBJDJJGMGHKQ
245	21.69	C ₃₀ H ₃₈ O ₄	463.2847	1	225.16	445.2741,417.2771,231.1 387,185.1334,177.0923,1 63.0762	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpeno id	MI- CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N RBJDJJGMGHKQ
246	22.04	C ₃₀ H ₃₈ O ₄	463.285	1.5	213.4	389.2492,325.1735,231.1 385,175.0764,173.0973	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpeno id	MI- CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N DJINKBUXGFQI
247	22.33	C ₃₄ H ₄₂ O ₈	579.2927	-4.5	243.87	561.2827,495.2665,372.1 176,260.1730,184.0740	biatractylenolide II or its isomer	5	Sesquiterpeno id	CR- GJDTUZTCSA-N

248	22.37	C ₃₀ H ₃₈ O ₄	463.2854	1.9	219.87	447.2905,231.1388,213.1 283,185.1335,163.0762,1 43.0859,105.0705	biatractylenolide/biepiasterolide	1	Sesquiterpeno id	RBJDJJGMGHKQ MI- CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N
249	22.47	C ₃₀ H ₃₈ O ₄	463.2852	1.9	227.46	417.1962,287.1659,229.1 235,185.1335	biatractylenolide/biepiasterolide or isomer	1	Sesquiterpeno id	RBJDJJGMGHKQ MI- CKRYVEOESA- N/OMASYMUHH SLTOE- PZGFELFZSA-N
250	22.82	C ₁₅ H ₁₈ O ₂	231.1385	2.2	152.25	213.1282,185.0974,155.0 860,141.0704,128.0625,1 15.0548	isomer of atractylenolide I	1	Sesquiterpeno id	-
251	22.84	C ₁₇ H ₂₂ O ₂	259.1703	4	161.97	259.1696,243.1389,203.1 436	2-dimethyl-octadienyl-methyl- cyclohexadiene-1,4-dione or its isomer	1	Benzoquinone	VDDALGSXMJY SIM- MDWZMJQESA- N

^a The compounds identified by comparison with the reference standards.